Full wwPDB X-ray Structure Validation Report

Sep 25, 2023 – 10:48 PM EDT

PDB ID	:	6BF4
Title	:	Crystal Structure of HIV-1 Clade AE Strain CNE55 gp120 Core in Complex with Neutralizing Antibody VRC-PG05 that Targets the Center of the Silent Face on the Outer Domain of gp120
Authors	:	Zhou, T.; Kwong, P.D.
Deposited on	:	2017-10-25
Resolution	:	2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

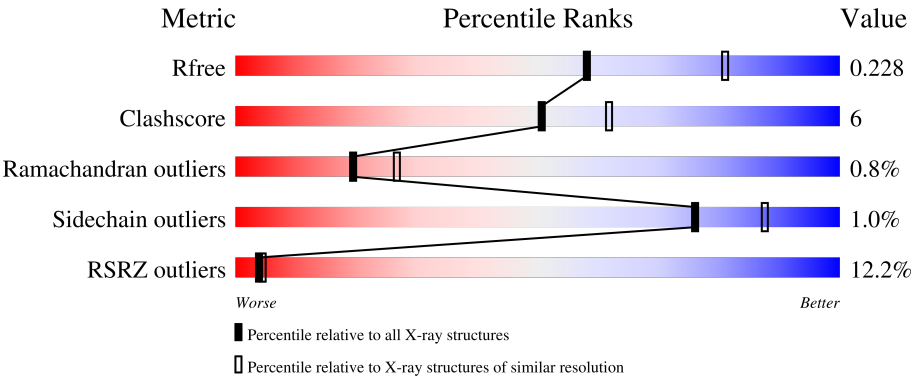
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	26% 80% 17%
1	G	344	10% 84% 12%
2	B	229	9% 76% 21%
2	H	229	8% 82% 15%
3	C	219	5% 89% 11%

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Mol	Chain	Length	Quality of chain
3	L	219	8% 86% 13%
4	D	10	20% 80%
5	E	2	100%
6	F	6	33% 67%
7	I	9	11% 89%
7	N	9	22% 78%
8	J	11	18% 82%
9	K	5	60% 40%
10	M	5	40% 60%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	A	524	-	-	-	X
11	NAG	G	502	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 13124 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 clade AE gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2639	1656	460	503	20			
1	G	333	Total	C	N	O	S	0	0	0
			2607	1639	452	496	20			

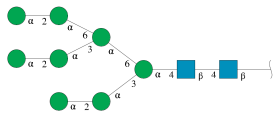
- Molecule 2 is a protein called VRC-PG05 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1702	1077	290	326	9			
2	H	221	Total	C	N	O	S	0	0	0
			1676	1062	285	320	9			

- Molecule 3 is a protein called VRC-PG05 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1714	1077	291	340	6			
3	L	218	Total	C	N	O	S	0	0	0
			1707	1074	290	338	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

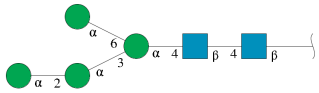


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	10	Total C N O 116 64 2 50	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

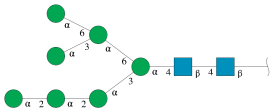
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	6	Total C N O 72 40 2 30	0	0	0

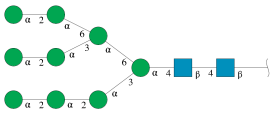
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	I	9	Total C N O 105 58 2 45	0	0	0
7	N	9	Total C N O 105 58 2 45	0	0	0

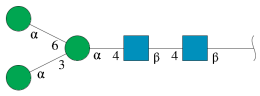
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



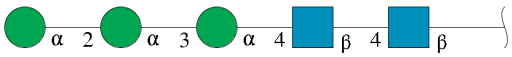
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



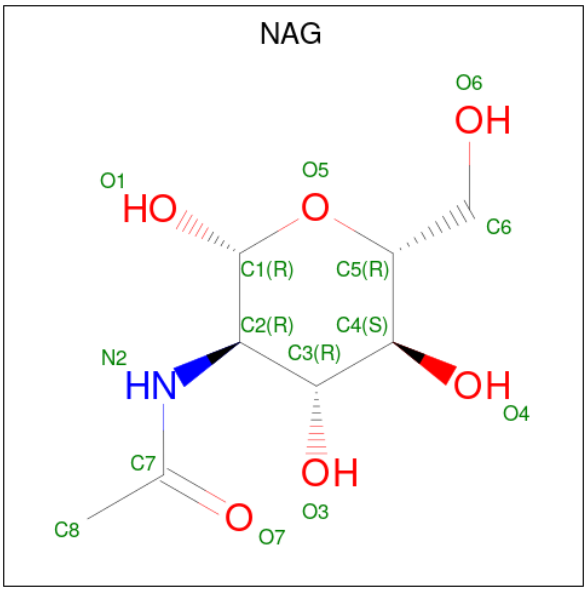
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



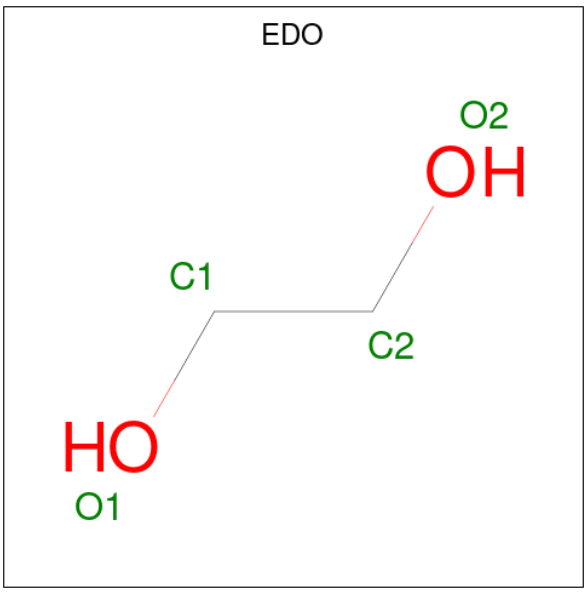
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



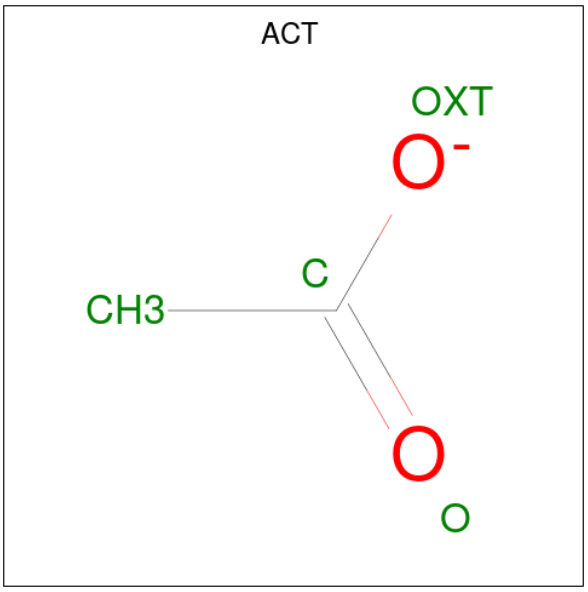
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	A	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	G	1	Total C N O 14 8 1 5	0	0
11	L	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	H	1	Total	C	O	0	0
			4	2	2		
12	L	1	Total	C	O	0	0
			4	2	2		
12	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 4 2 2	0	0

- Molecule 14 is water.

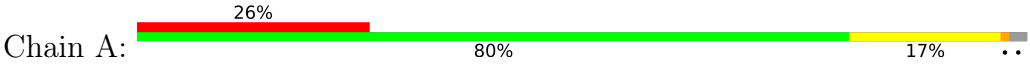
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	7	Total O 7 7	0	0
14	B	26	Total O 26 26	0	0
14	C	30	Total O 30 30	0	0
14	G	36	Total O 36 36	0	0
14	H	38	Total O 38 38	0	0
14	L	39	Total O 39 39	0	0

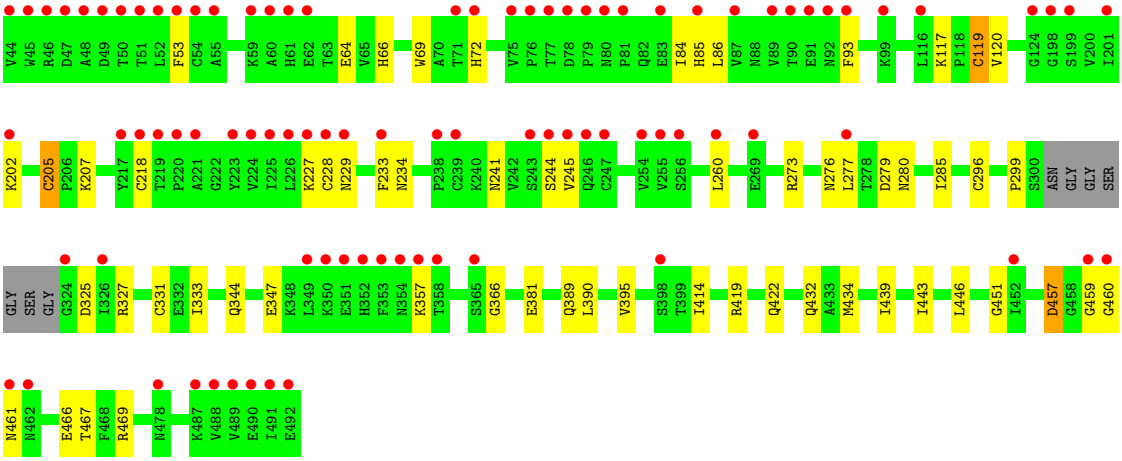
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HIV-1 clade AE gp120 core

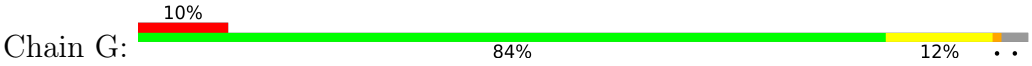
Chain A:

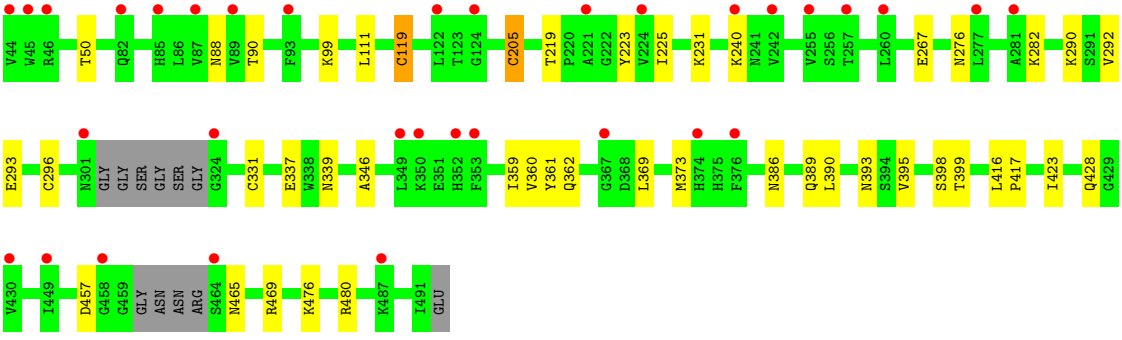




• Molecule 1: HIV-1 clade AE gp120 core

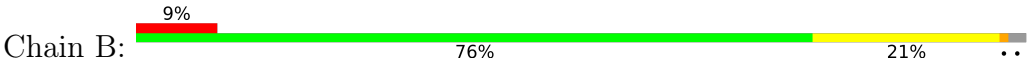
Chain G:

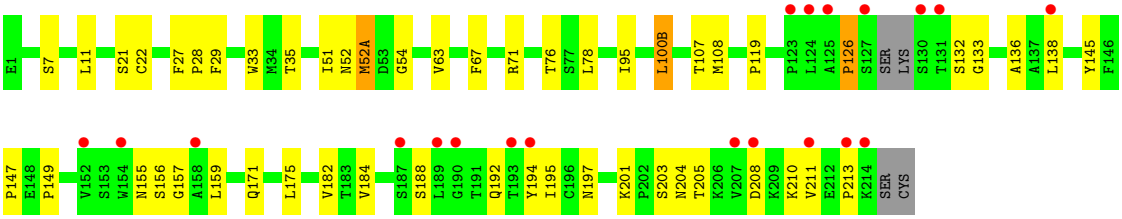




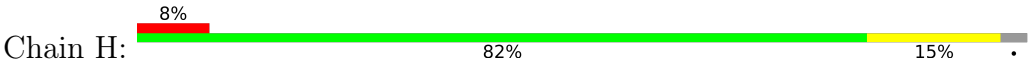
• Molecule 2: VRC-PG05 Fab heavy chain

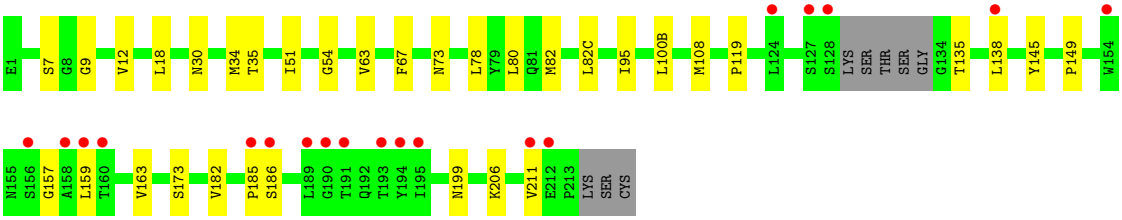
Chain B:



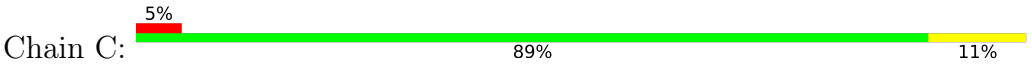


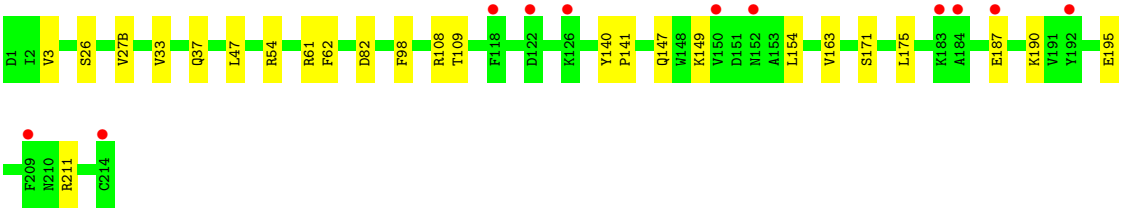
• Molecule 2: VRC-PG05 Fab heavy chain



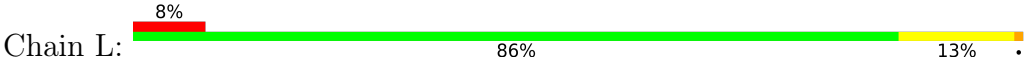


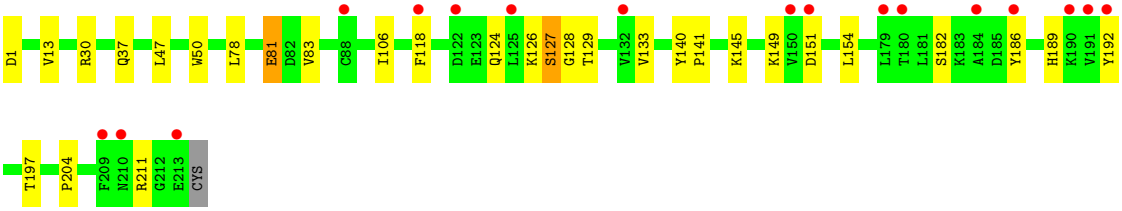
• Molecule 3: VRC-PG05 Fab light chain



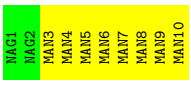


• Molecule 3: VRC-PG05 Fab light chain



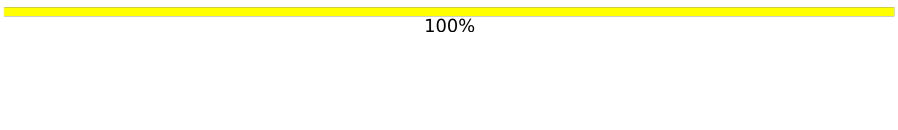


• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

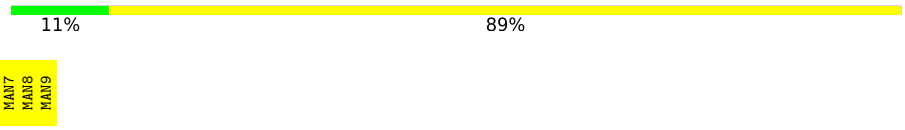


• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

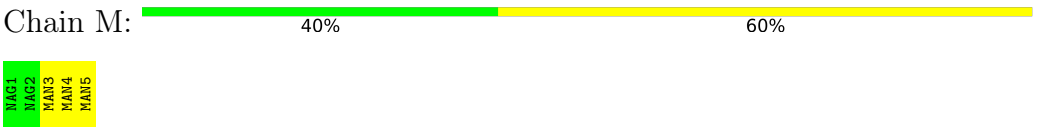
Chain J:

• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.44Å 89.25Å 123.41Å 90.00° 119.15° 90.00°	Depositor
Resolution (Å)	39.85 – 2.38 39.85 – 2.38	Depositor EDS
% Data completeness (in resolution range)	88.5 (39.85-2.38) 88.5 (39.85-2.38)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.192 , 0.228 0.192 , 0.228	Depositor DCC
R_{free} test set	3888 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, ACT, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/2696	0.43	0/3661
1	G	0.25	0/2663	0.44	0/3616
2	B	0.25	0/1743	0.49	0/2370
2	H	0.26	0/1717	0.49	0/2336
3	C	0.25	0/1755	0.45	0/2383
3	L	0.26	0/1748	0.47	0/2375
All	All	0.25	0/12322	0.46	0/16741

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2569	39	0
1	G	2607	0	2540	27	0
2	B	1702	0	1677	29	0
2	H	1676	0	1649	16	0
3	C	1714	0	1647	17	0
3	L	1707	0	1642	18	0
4	D	116	0	97	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	25	3	0
6	F	72	0	61	1	0
7	I	105	0	88	1	0
7	N	105	0	88	0	0
8	J	127	0	106	0	0
9	K	61	0	52	0	0
10	M	61	0	52	0	0
11	A	84	0	78	3	0
11	C	14	0	13	0	0
11	G	84	0	78	1	0
11	L	14	0	13	0	0
12	A	4	0	6	0	0
12	B	8	0	12	3	0
12	G	4	0	6	2	0
12	H	4	0	6	0	0
12	L	8	0	12	0	0
13	B	4	0	3	0	0
14	A	7	0	0	0	0
14	B	26	0	0	0	0
14	C	30	0	0	0	0
14	G	36	0	0	0	0
14	H	38	0	0	0	0
14	L	39	0	0	1	0
All	All	13124	0	12520	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:189:HIS:O	3:L:211:ARG:NH1	2.05	0.90
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.55	0.86
1:A:357:LYS:NZ	1:A:461:ASN:O	2.07	0.86
1:G:50:THR:O	1:G:99:LYS:NZ	2.10	0.84
1:G:389:GLN:HB3	11:G:527:NAG:H61	1.62	0.82
3:C:187:GLU:O	3:C:211:ARG:NH1	2.15	0.80
1:A:432:GLN:HG2	1:G:423:ILE:HD11	1.69	0.75
2:B:201:LYS:HD2	12:B:302:EDO:H11	1.75	0.69
1:A:227:LYS:HE3	1:A:245:VAL:HG11	1.75	0.68
3:L:126:LYS:O	3:L:128:GLY:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:ARG:NH1	3:C:62:PHE:O	2.26	0.67
1:G:361:TYR:N	1:G:393:ASN:OD1	2.24	0.66
1:G:292:VAL:HG13	12:G:537:EDO:H11	1.78	0.65
1:A:461:ASN:ND2	1:A:466:GLU:OE2	2.31	0.63
1:G:339:ASN:HD22	1:G:395:VAL:HB	1.65	0.62
2:B:197:ASN:ND2	2:B:208:ASP:OD2	2.34	0.61
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.82	0.60
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.82	0.60
3:L:126:LYS:HG3	3:L:127:SER:H	1.66	0.59
1:G:390:LEU:HD13	1:G:416:LEU:HD21	1.83	0.59
1:G:119:CYS:N	1:G:205:CYS:SG	2.76	0.59
1:A:64:GLU:OE2	1:A:66:HIS:HD2	1.87	0.57
2:B:52:ASN:O	2:B:71:ARG:NH2	2.37	0.57
2:B:100(B):LEU:HB2	7:I:1:NAG:HN2	1.69	0.57
2:B:188:SER:HB3	2:B:192:GLN:HB3	1.85	0.57
3:C:61:ARG:HH12	3:C:82:ASP:CG	2.05	0.57
1:G:293:GLU:H	12:G:537:EDO:H12	1.69	0.57
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.85	0.57
3:L:83:VAL:HB	3:L:106:ILE:HD13	1.85	0.57
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.87	0.56
3:L:149:LYS:HG2	3:L:154:LEU:HD23	1.88	0.56
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.88	0.56
3:C:61:ARG:NH1	3:C:82:ASP:OD1	2.25	0.55
2:H:135:THR:HA	2:H:185:PRO:HA	1.89	0.55
2:H:138:LEU:HD13	2:H:211:VAL:HG21	1.87	0.55
1:G:290:LYS:NZ	1:G:337:GLU:HG3	2.22	0.55
2:B:35:THR:HB	2:B:95:ILE:HD11	1.88	0.54
2:B:136:ALA:N	2:B:184:VAL:O	2.33	0.54
1:A:277:LEU:HD11	11:A:501:NAG:H83	1.88	0.54
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.89	0.54
1:G:90:THR:HG22	1:G:240:LYS:HA	1.90	0.54
2:H:199:ASN:ND2	2:H:206:LYS:HE2	2.23	0.53
3:C:147:GLN:HB3	3:C:195:GLU:HB3	1.90	0.53
1:A:229:ASN:HB2	1:A:241:ASN:HB3	1.90	0.53
2:B:107:THR:HG22	12:B:302:EDO:H12	1.91	0.53
2:B:159:LEU:HD13	2:B:182:VAL:HG21	1.91	0.52
1:A:389:GLN:HB3	11:A:523:NAG:H61	1.91	0.52
3:C:27(B):VAL:HG21	3:C:33:VAL:HG23	1.90	0.52
1:A:347:GLU:HG2	5:E:2:NAG:H83	1.92	0.52
1:A:459:GLY:O	1:A:461:ASN:N	2.43	0.52
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:LYS:HB2	3:C:190:LYS:NZ	2.24	0.52
1:G:369:LEU:HD22	1:G:373:MET:HE2	1.92	0.52
1:G:386:ASN:HB3	1:G:417:PRO:HG2	1.91	0.52
1:A:327:ARG:NH1	1:A:422:GLN:OE1	2.43	0.51
2:B:203:SER:O	2:B:205:THR:N	2.43	0.51
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.46	0.51
3:L:186:TYR:O	3:L:192:TYR:OH	2.27	0.51
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.93	0.51
3:L:129:THR:HA	3:L:182:SER:HA	1.94	0.50
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.94	0.50
1:G:290:LYS:HZ1	1:G:337:GLU:HG3	1.77	0.50
2:H:159:LEU:HD21	2:H:182:VAL:HG11	1.93	0.50
2:B:108:MET:HB3	2:B:149:PRO:HD3	1.94	0.49
3:C:108:ARG:HD2	3:C:171:SER:HB2	1.93	0.49
1:G:398:SER:OG	1:G:399:THR:N	2.45	0.49
1:A:381:GLU:OE2	1:A:439:ILE:HG23	2.12	0.49
3:C:3:VAL:H	3:C:26:SER:HB3	1.78	0.49
3:L:30:ARG:HD2	3:L:50:TRP:CE3	2.48	0.49
1:A:446:LEU:HD22	6:F:1:NAG:H82	1.95	0.48
2:B:171:GLN:HG2	2:B:175:LEU:O	2.13	0.48
3:C:108:ARG:NH1	3:C:109:THR:O	2.46	0.48
3:C:163:VAL:HG22	3:C:175:LEU:HD12	1.96	0.48
3:C:61:ARG:NH1	3:C:82:ASP:OD2	2.47	0.47
3:C:140:TYR:CG	3:C:141:PRO:HA	2.49	0.47
2:B:126:PRO:HG3	2:B:138:LEU:HD23	1.94	0.47
1:G:219:THR:OG1	1:G:225:ILE:HG13	2.14	0.47
1:G:231:LYS:HG2	1:G:267:GLU:OE2	2.15	0.47
3:L:1:ASP:HB2	14:L:414:HOH:O	2.14	0.47
3:C:61:ARG:NH1	3:C:82:ASP:CG	2.67	0.47
2:H:35:THR:HB	2:H:95:ILE:HD11	1.96	0.46
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.98	0.46
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.51	0.46
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.97	0.46
2:H:108:MET:HB3	2:H:149:PRO:HD3	1.96	0.46
1:A:119:CYS:N	1:A:205:CYS:SG	2.89	0.46
2:H:163:VAL:HG22	2:H:182:VAL:HG22	1.98	0.46
2:B:132:SER:OG	2:B:133:GLY:N	2.49	0.45
2:B:155:ASN:O	2:B:157:GLY:N	2.49	0.45
1:A:296:CYS:HA	1:A:331:CYS:HA	1.98	0.45
1:A:53:PHE:CE1	1:A:218:CYS:HB2	2.51	0.45
1:A:395:VAL:HG13	1:A:414:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE2	1:A:66:HIS:CD2	2.69	0.45
3:L:124:GLN:O	3:L:127:SER:OG	2.30	0.45
3:L:145:LYS:HE3	3:L:145:LYS:HB3	1.87	0.45
1:A:325:ASP:OD2	1:A:419:ARG:NH1	2.50	0.45
1:A:344:GLN:HA	5:E:2:NAG:H81	1.97	0.44
2:B:33:TRP:HB2	2:B:95:ILE:HB	1.99	0.44
1:A:202:LYS:HB3	1:A:202:LYS:HE2	1.69	0.44
2:B:138:LEU:HD21	2:B:194:TYR:CD2	2.53	0.44
3:L:13:VAL:HB	3:L:78:LEU:HD22	1.99	0.44
1:A:84:ILE:O	1:A:86:LEU:N	2.50	0.44
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.18	0.44
3:C:149:LYS:HG2	3:C:154:LEU:HD13	2.00	0.44
1:G:476:LYS:O	1:G:480:ARG:HG3	2.17	0.44
2:H:12:VAL:HG11	2:H:82(C):LEU:HD12	2.00	0.43
3:L:140:TYR:CG	3:L:141:PRO:HA	2.53	0.43
1:G:362:GLN:O	1:G:469:ARG:HG2	2.17	0.43
2:H:12:VAL:HG21	2:H:18:LEU:HD22	2.00	0.43
1:G:360:VAL:HG21	1:G:465:ASN:HD22	1.82	0.43
3:L:81:GLU:H	3:L:81:GLU:HG3	1.42	0.43
1:A:457:ASP:OD2	1:A:469:ARG:NE	2.38	0.43
1:G:296:CYS:HA	1:G:331:CYS:HA	2.00	0.43
2:B:52(A):MET:SD	2:B:52(A):MET:N	2.82	0.43
1:A:69:TRP:HA	1:A:72:HIS:CE1	2.53	0.43
1:A:84:ILE:HB	1:A:244:SER:HB2	2.00	0.43
2:B:51:ILE:HD11	2:B:54:GLY:HA2	2.00	0.43
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.99	0.43
3:L:151:ASP:OD2	3:L:189:HIS:HB3	2.18	0.43
1:A:120:VAL:HB	1:A:434:MET:HE3	2.00	0.42
2:H:30:ASN:HB3	2:H:73:ASN:HB3	2.01	0.42
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.01	0.42
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.83	0.42
12:B:301:EDO:H21	3:C:98:PHE:H	1.84	0.42
1:G:282:LYS:HD3	1:G:282:LYS:HA	1.90	0.42
1:G:428:GLN:OE1	1:G:428:GLN:N	2.38	0.41
1:A:234:ASN:HD22	11:A:501:NAG:C7	2.32	0.41
1:G:346:ALA:O	1:G:359:ILE:HG13	2.20	0.41
1:A:276:ASN:ND2	1:A:279:ASP:HB2	2.34	0.41
1:G:339:ASN:ND2	1:G:395:VAL:HB	2.34	0.41
2:B:11:LEU:HB2	2:B:147:PRO:HG3	2.01	0.41
1:G:219:THR:HG21	1:G:223:TYR:C	2.41	0.41
2:B:7:SER:HB3	2:B:21:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HB2	1:A:285:ILE:HB	2.02	0.41
1:A:333:ILE:HG21	1:A:390:LEU:HD21	2.03	0.41
2:B:126:PRO:HD2	2:B:213:PRO:HA	2.03	0.41
2:B:138:LEU:HB2	2:B:211:VAL:HG11	2.03	0.41
2:B:27:PHE:O	2:B:29:PHE:N	2.54	0.41
5:E:1:NAG:H62	5:E:2:NAG:N2	2.36	0.40
1:A:93:PHE:CE1	1:A:228:CYS:HB2	2.55	0.40
2:B:29:PHE:CD1	2:B:76:THR:HA	2.56	0.40
1:A:207:LYS:HG3	1:A:439:ILE:HG22	2.03	0.40
2:B:195:ILE:HG22	2:B:210:LYS:HA	2.02	0.40
1:A:457:ASP:HB2	1:A:467:THR:HB	2.03	0.40
1:G:457:ASP:OD1	1:G:469:ARG:NH2	2.55	0.40
2:H:80:LEU:HD23	2:H:82:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	303 (91%)	25 (8%)	5 (2%)	10 12
1	G	327/344 (95%)	312 (95%)	14 (4%)	1 (0%)	41 53
2	B	221/229 (96%)	200 (90%)	17 (8%)	4 (2%)	8 9
2	H	217/229 (95%)	203 (94%)	12 (6%)	2 (1%)	17 23
3	C	217/219 (99%)	207 (95%)	10 (5%)	0	100 100
3	L	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	29 39
All	All	1531/1584 (97%)	1432 (94%)	86 (6%)	13 (1%)	19 27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
3	L	127	SER
1	A	460	GLY
2	B	126	PRO
1	A	85	HIS
1	A	280	ASN
2	B	156	SER
1	A	299	PRO
1	G	276	ASN
2	H	157	GLY
2	H	186	SER
2	B	28	PRO
1	A	366	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	299/302 (99%)	296 (99%)	3 (1%)	76 87
1	G	296/302 (98%)	292 (99%)	4 (1%)	67 81
2	B	189/193 (98%)	187 (99%)	2 (1%)	73 86
2	H	186/193 (96%)	183 (98%)	3 (2%)	62 78
3	C	193/193 (100%)	193 (100%)	0	100 100
3	L	192/193 (100%)	191 (100%)	1 (0%)	88 95
All	All	1355/1376 (98%)	1342 (99%)	13 (1%)	76 87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	CYS
1	A	205	CYS
1	A	457	ASP
2	B	52(A)	MET
2	B	100(B)	LEU
1	G	88	ASN

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Mol	Chain	Res	Type
1	G	111	LEU
1	G	119	CYS
1	G	205	CYS
2	H	7	SER
2	H	100(B)	LEU
2	H	173	SER
3	L	81	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

57 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.32	0	17,19,21	0.52	0
4	MAN	D	10	4	11,11,12	0.67	0	15,15,17	1.37	2 (13%)
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	MAN	D	3	4	11,11,12	0.74	0	15,15,17	0.99	1 (6%)
4	MAN	D	4	4	11,11,12	0.55	0	15,15,17	1.18	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	D	5	4	11,11,12	0.73	0	15,15,17	1.42	2 (13%)
4	MAN	D	6	4	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
4	MAN	D	7	4	11,11,12	0.73	0	15,15,17	1.26	2 (13%)
4	MAN	D	8	4	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
4	MAN	D	9	4	11,11,12	0.66	0	15,15,17	1.14	1 (6%)
5	NAG	E	1	5,1	14,14,15	0.23	0	17,19,21	0.60	0
5	NAG	E	2	5	14,14,15	0.25	0	17,19,21	0.51	0
6	NAG	F	1	6,1	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.30	0	17,19,21	0.54	0
6	MAN	F	3	6	11,11,12	0.78	0	15,15,17	0.98	0
6	MAN	F	4	6	11,11,12	0.66	0	15,15,17	1.12	1 (6%)
6	MAN	F	5	6	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
6	MAN	F	6	6	11,11,12	0.73	0	15,15,17	1.02	2 (13%)
7	NAG	I	1	7,1	14,14,15	0.17	0	17,19,21	0.62	0
7	NAG	I	2	7	14,14,15	0.28	0	17,19,21	0.48	0
7	MAN	I	3	7	11,11,12	0.76	0	15,15,17	1.00	2 (13%)
7	MAN	I	4	7	11,11,12	1.09	2 (18%)	15,15,17	1.08	0
7	MAN	I	5	7	11,11,12	0.73	0	15,15,17	1.24	2 (13%)
7	MAN	I	6	7	11,11,12	0.76	0	15,15,17	0.98	2 (13%)
7	MAN	I	7	7	11,11,12	0.71	0	15,15,17	1.32	2 (13%)
7	MAN	I	8	7	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
7	MAN	I	9	7	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
8	NAG	J	1	8,1	14,14,15	0.25	0	17,19,21	0.49	0
8	MAN	J	10	8	11,11,12	0.85	0	15,15,17	1.00	1 (6%)
8	MAN	J	11	8	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
8	NAG	J	2	8	14,14,15	0.41	0	17,19,21	0.56	0
8	MAN	J	3	8	11,11,12	0.82	1 (9%)	15,15,17	1.32	2 (13%)
8	MAN	J	4	8	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
8	MAN	J	5	8	11,11,12	0.74	0	15,15,17	1.36	3 (20%)
8	MAN	J	6	8	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
8	MAN	J	7	8	11,11,12	0.62	0	15,15,17	1.14	2 (13%)
8	MAN	J	8	8	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
8	MAN	J	9	8	11,11,12	0.78	0	15,15,17	1.13	2 (13%)
9	NAG	K	1	9,1	14,14,15	0.21	0	17,19,21	0.40	0
9	NAG	K	2	9	14,14,15	0.23	0	17,19,21	0.62	0
9	MAN	K	3	9	11,11,12	1.08	0	15,15,17	0.78	0
9	MAN	K	4	9	11,11,12	1.25	2 (18%)	15,15,17	1.51	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	K	5	9	11,11,12	1.01	1 (9%)	15,15,17	1.24	2 (13%)
10	NAG	M	1	10,1	14,14,15	0.37	0	17,19,21	0.48	0
10	NAG	M	2	10	14,14,15	0.27	0	17,19,21	0.57	0
10	MAN	M	3	10	11,11,12	0.95	0	15,15,17	0.91	1 (6%)
10	MAN	M	4	10	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
10	MAN	M	5	10	11,11,12	0.79	1 (9%)	15,15,17	1.14	2 (13%)
7	NAG	N	1	7,1	14,14,15	0.43	0	17,19,21	0.58	0
7	NAG	N	2	7	14,14,15	0.29	0	17,19,21	0.50	0
7	MAN	N	3	7	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
7	MAN	N	4	7	11,11,12	1.00	1 (9%)	15,15,17	0.93	0
7	MAN	N	5	7	11,11,12	0.85	0	15,15,17	1.21	2 (13%)
7	MAN	N	6	7	11,11,12	0.80	0	15,15,17	0.99	2 (13%)
7	MAN	N	7	7	11,11,12	0.91	1 (9%)	15,15,17	1.01	1 (6%)
7	MAN	N	8	7	11,11,12	0.77	0	15,15,17	0.93	1 (6%)
7	MAN	N	9	7	11,11,12	0.68	0	15,15,17	1.01	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	MAN	D	10	4	-	0/2/19/22	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	1/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
4	MAN	D	8	4	-	1/2/19/22	0/1/1/1
4	MAN	D	9	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	MAN	F	3	6	-	2/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	1/2/19/22	0/1/1/1
7	NAG	I	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	MAN	I	3	7	-	2/2/19/22	1/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	1/2/19/22	0/1/1/1
7	MAN	I	6	7	-	1/2/19/22	0/1/1/1
7	MAN	I	7	7	-	0/2/19/22	0/1/1/1
7	MAN	I	8	7	-	0/2/19/22	0/1/1/1
7	MAN	I	9	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	MAN	J	10	8	-	0/2/19/22	0/1/1/1
8	MAN	J	11	8	-	1/2/19/22	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	MAN	J	3	8	-	2/2/19/22	1/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	2/2/19/22	0/1/1/1
8	MAN	J	6	8	-	0/2/19/22	0/1/1/1
8	MAN	J	7	8	-	0/2/19/22	0/1/1/1
8	MAN	J	8	8	-	0/2/19/22	0/1/1/1
8	MAN	J	9	8	-	0/2/19/22	0/1/1/1
9	NAG	K	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	MAN	K	3	9	-	2/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	0/2/19/22	1/1/1/1
10	NAG	M	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	MAN	M	3	10	-	2/2/19/22	1/1/1/1
10	MAN	M	4	10	-	2/2/19/22	0/1/1/1
10	MAN	M	5	10	-	0/2/19/22	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	MAN	N	3	7	-	2/2/19/22	0/1/1/1
7	MAN	N	4	7	-	1/2/19/22	0/1/1/1
7	MAN	N	5	7	-	0/2/19/22	0/1/1/1
7	MAN	N	6	7	-	0/2/19/22	0/1/1/1
7	MAN	N	7	7	-	0/2/19/22	0/1/1/1
7	MAN	N	8	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	N	9	7	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	4	MAN	C4-C5	2.75	1.58	1.53
9	K	5	MAN	C1-C2	2.61	1.58	1.52
9	K	4	MAN	O5-C5	2.38	1.48	1.43
7	N	7	MAN	O5-C1	-2.35	1.40	1.43
7	I	4	MAN	C2-C3	2.26	1.55	1.52
7	N	4	MAN	O5-C1	-2.17	1.40	1.43
8	J	3	MAN	O5-C5	2.14	1.47	1.43
10	M	5	MAN	C1-C2	2.05	1.56	1.52
7	I	4	MAN	C1-C2	2.02	1.56	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5	MAN	C1-O5-C5	4.40	118.15	112.19
4	D	10	MAN	C1-O5-C5	4.25	117.95	112.19
9	K	4	MAN	C1-O5-C5	3.89	117.47	112.19
8	J	6	MAN	C1-O5-C5	3.72	117.23	112.19
8	J	3	MAN	C1-O5-C5	3.58	117.05	112.19
9	K	5	MAN	C1-O5-C5	3.56	117.01	112.19
8	J	5	MAN	C1-O5-C5	3.49	116.92	112.19
8	J	8	MAN	C1-O5-C5	3.47	116.89	112.19
4	D	7	MAN	C1-O5-C5	3.32	116.69	112.19
10	M	4	MAN	C1-O5-C5	3.28	116.64	112.19
7	I	5	MAN	O2-C2-C3	-3.25	103.62	110.14
6	F	4	MAN	C1-O5-C5	3.23	116.56	112.19
4	D	4	MAN	C1-O5-C5	3.18	116.51	112.19
8	J	10	MAN	O2-C2-C3	-3.15	103.83	110.14
7	I	8	MAN	C1-O5-C5	3.14	116.45	112.19
10	M	5	MAN	C1-O5-C5	3.05	116.32	112.19
4	D	9	MAN	C1-O5-C5	3.03	116.29	112.19
7	I	5	MAN	C1-O5-C5	2.98	116.23	112.19
6	F	5	MAN	C1-O5-C5	2.92	116.14	112.19
4	D	7	MAN	O2-C2-C3	-2.91	104.31	110.14
8	J	8	MAN	O2-C2-C3	-2.86	104.41	110.14
7	I	7	MAN	C1-O5-C5	2.86	116.07	112.19
7	N	5	MAN	O2-C2-C3	-2.82	104.49	110.14
8	J	7	MAN	C1-O5-C5	2.81	116.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	5	MAN	C1-O5-C5	2.80	115.99	112.19
8	J	4	MAN	C1-O5-C5	2.79	115.97	112.19
7	I	9	MAN	C1-O5-C5	2.76	115.94	112.19
8	J	9	MAN	C1-O5-C5	2.76	115.93	112.19
6	F	6	MAN	C1-O5-C5	2.71	115.86	112.19
7	N	9	MAN	C1-O5-C5	2.70	115.85	112.19
8	J	9	MAN	O2-C2-C3	-2.65	104.83	110.14
7	I	7	MAN	O2-C2-C3	-2.65	104.84	110.14
4	D	3	MAN	C1-O5-C5	2.62	115.74	112.19
4	D	5	MAN	O2-C2-C3	-2.61	104.90	110.14
9	K	4	MAN	C3-C4-C5	2.60	114.87	110.24
4	D	4	MAN	O2-C2-C3	-2.59	104.96	110.14
4	D	8	MAN	O2-C2-C3	-2.58	104.98	110.14
7	N	3	MAN	C1-O5-C5	2.56	115.67	112.19
8	J	7	MAN	O2-C2-C3	-2.51	105.11	110.14
4	D	8	MAN	C1-O5-C5	2.51	115.59	112.19
8	J	11	MAN	O2-C2-C3	-2.51	105.12	110.14
7	N	6	MAN	C1-O5-C5	2.50	115.58	112.19
7	I	3	MAN	C1-O5-C5	2.50	115.58	112.19
4	D	6	MAN	C1-O5-C5	2.46	115.53	112.19
7	N	7	MAN	O2-C2-C3	-2.44	105.25	110.14
7	N	3	MAN	O2-C2-C3	-2.44	105.25	110.14
8	J	5	MAN	C1-C2-C3	-2.43	106.68	109.67
8	J	4	MAN	O2-C2-C3	-2.35	105.43	110.14
8	J	11	MAN	C1-O5-C5	2.31	115.33	112.19
7	I	6	MAN	C1-O5-C5	2.30	115.31	112.19
7	I	8	MAN	O2-C2-C3	-2.28	105.57	110.14
7	I	9	MAN	O2-C2-C3	-2.24	105.65	110.14
4	D	10	MAN	O2-C2-C3	-2.24	105.66	110.14
7	I	3	MAN	O2-C2-C3	-2.20	105.73	110.14
8	J	3	MAN	C1-C2-C3	2.17	112.34	109.67
8	J	5	MAN	O2-C2-C3	-2.15	105.82	110.14
9	K	5	MAN	O2-C2-C3	-2.15	105.84	110.14
10	M	3	MAN	C1-O5-C5	2.14	115.09	112.19
7	N	6	MAN	O2-C2-C3	-2.14	105.85	110.14
7	I	6	MAN	O2-C2-C3	-2.13	105.87	110.14
4	D	6	MAN	O2-C2-C3	-2.12	105.90	110.14
7	N	8	MAN	O2-C2-C3	-2.11	105.91	110.14
6	F	6	MAN	O2-C2-C3	-2.09	105.96	110.14
10	M	5	MAN	O2-C2-C3	-2.06	106.01	110.14
6	F	5	MAN	O2-C2-C3	-2.06	106.01	110.14
10	M	4	MAN	O2-C2-C3	-2.03	106.08	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	6	MAN	O2-C2-C3	-2.01	106.11	110.14

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6	MAN	O5-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
6	F	3	MAN	C4-C5-C6-O6
7	N	3	MAN	C4-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
7	I	3	MAN	C4-C5-C6-O6
9	K	3	MAN	C4-C5-C6-O6
7	N	3	MAN	O5-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
7	I	3	MAN	O5-C5-C6-O6
9	K	1	NAG	C4-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
6	F	3	MAN	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
9	K	3	MAN	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
8	J	2	NAG	C8-C7-N2-C2
8	J	2	NAG	O7-C7-N2-C2
6	F	2	NAG	C4-C5-C6-O6
6	F	4	MAN	C4-C5-C6-O6
8	J	5	MAN	C4-C5-C6-O6
8	J	5	MAN	O5-C5-C6-O6
10	M	4	MAN	C4-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
8	J	3	MAN	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
8	J	3	MAN	O5-C5-C6-O6
4	D	9	MAN	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	N	9	MAN	C4-C5-C6-O6
6	F	6	MAN	O5-C5-C6-O6
7	N	9	MAN	O5-C5-C6-O6
10	M	4	MAN	O5-C5-C6-O6
8	J	11	MAN	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
7	I	6	MAN	C4-C5-C6-O6
10	M	3	MAN	O5-C5-C6-O6
10	M	3	MAN	C4-C5-C6-O6
4	D	8	MAN	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
6	F	1	NAG	O5-C5-C6-O6
7	N	4	MAN	O5-C5-C6-O6

All (5) ring outliers are listed below:

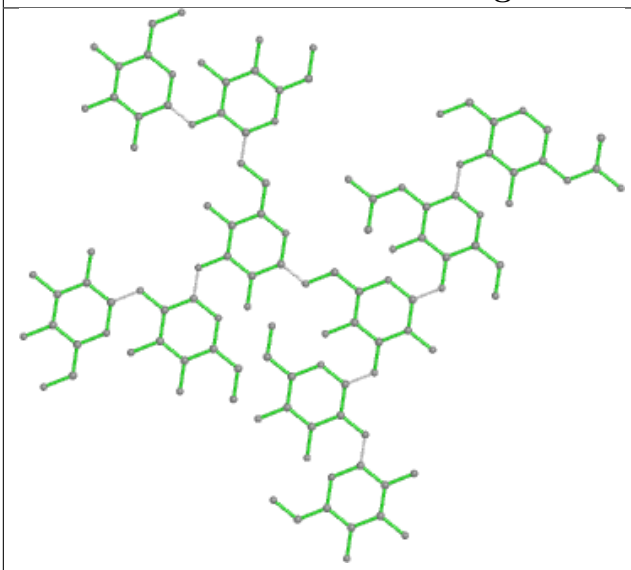
Mol	Chain	Res	Type	Atoms
9	K	5	MAN	C1-C2-C3-C4-C5-O5
7	I	3	MAN	C1-C2-C3-C4-C5-O5
10	M	3	MAN	C1-C2-C3-C4-C5-O5
8	J	3	MAN	C1-C2-C3-C4-C5-O5
4	D	3	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

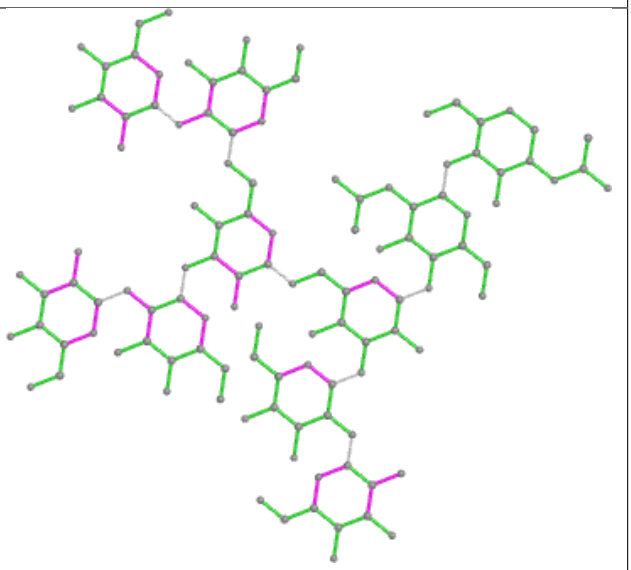
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	1	0
6	F	1	NAG	1	0
5	E	2	NAG	3	0
7	I	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

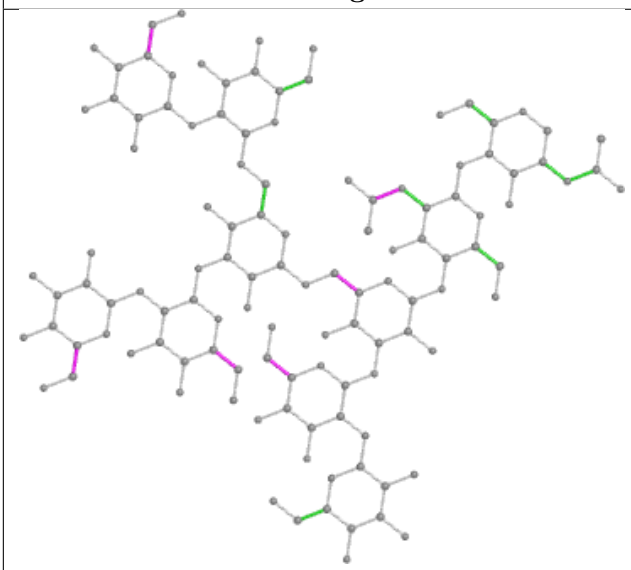
Oligosaccharide Chain D



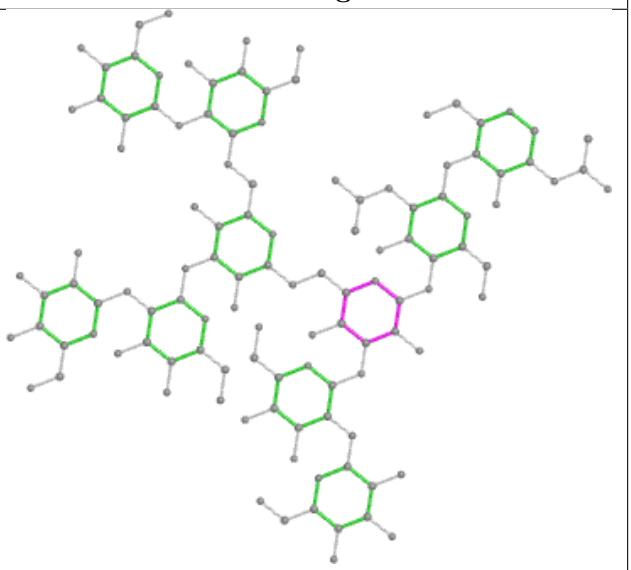
Bond lengths



Bond angles

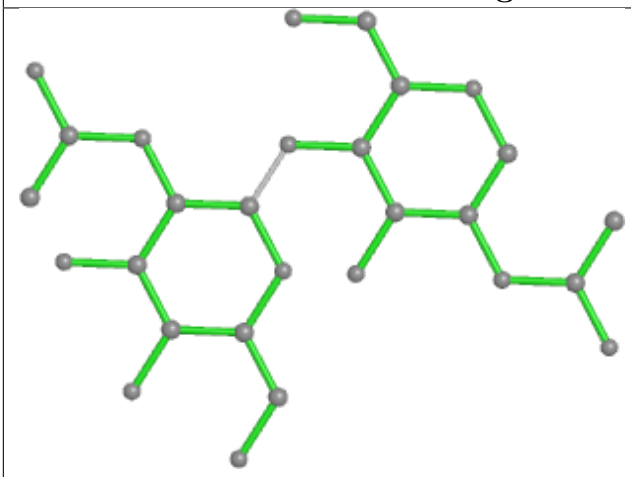


Torsions

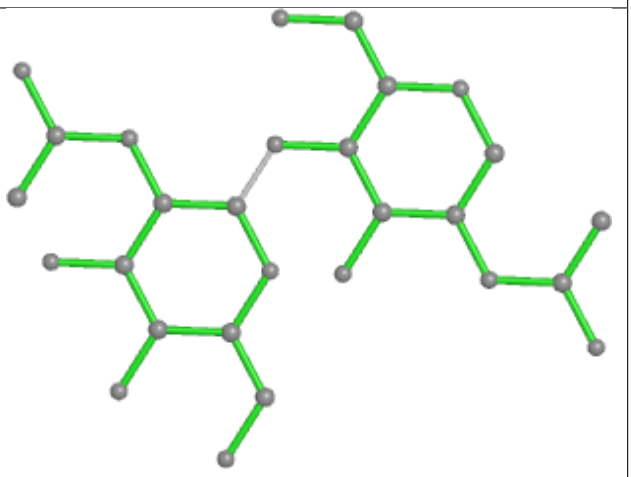


Rings

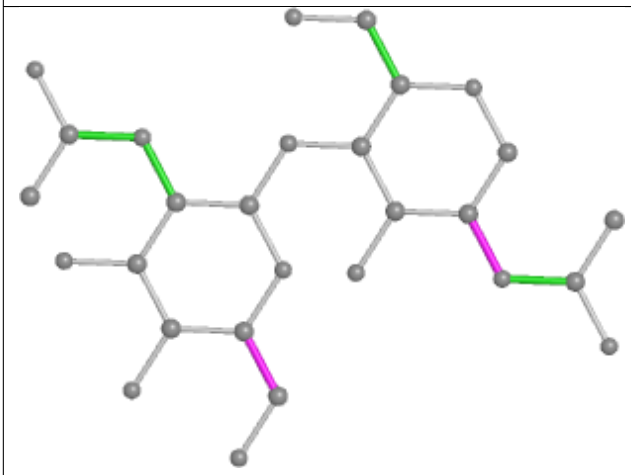
Oligosaccharide Chain E



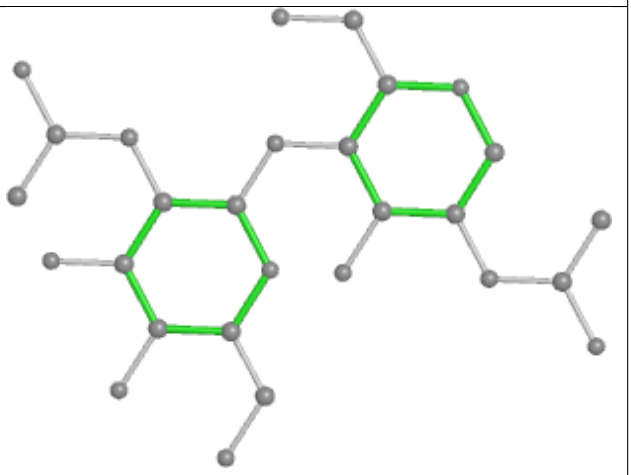
Bond lengths



Bond angles

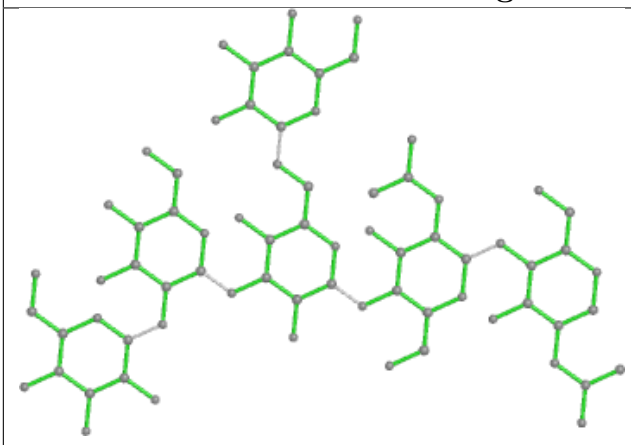


Torsions

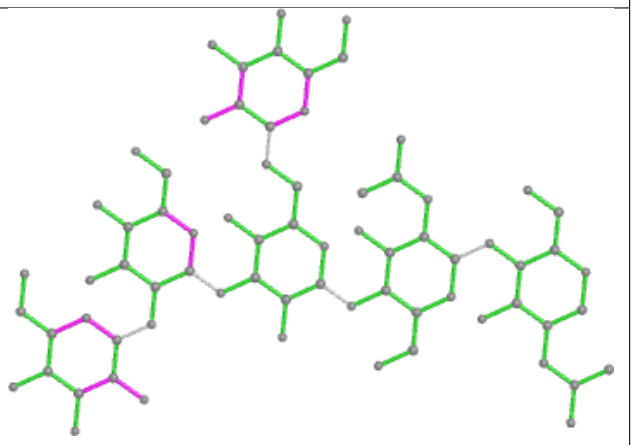


Rings

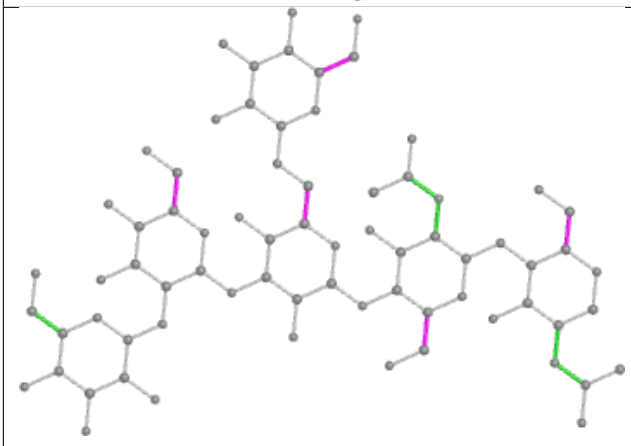
Oligosaccharide Chain F



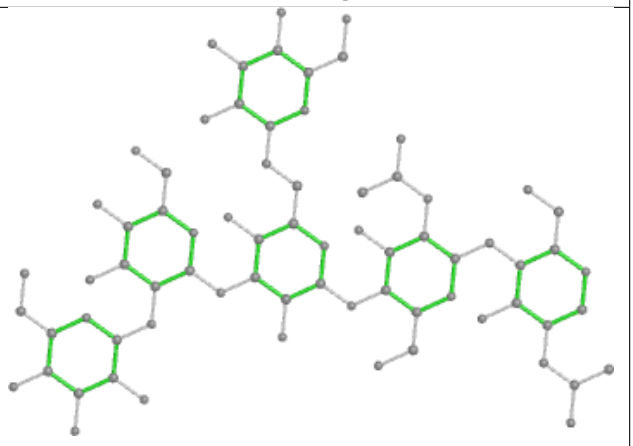
Bond lengths



Bond angles

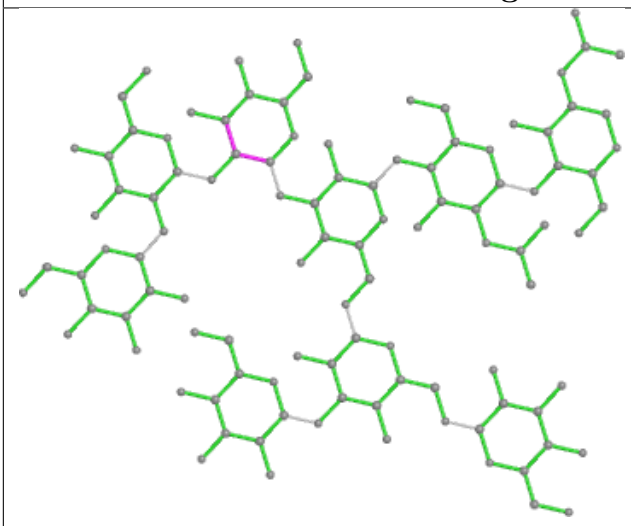


Torsions

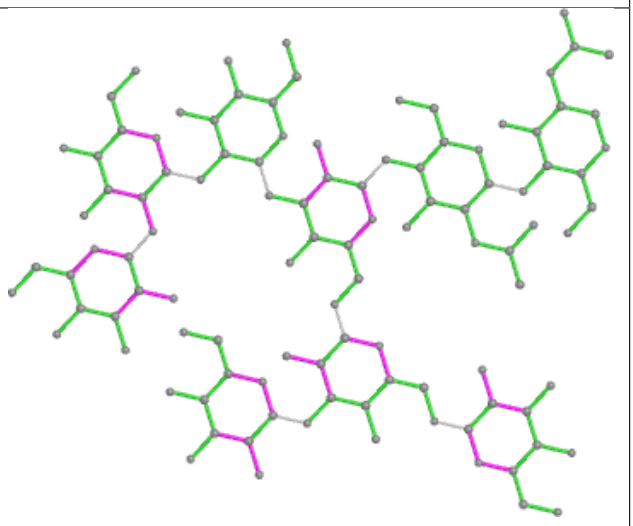


Rings

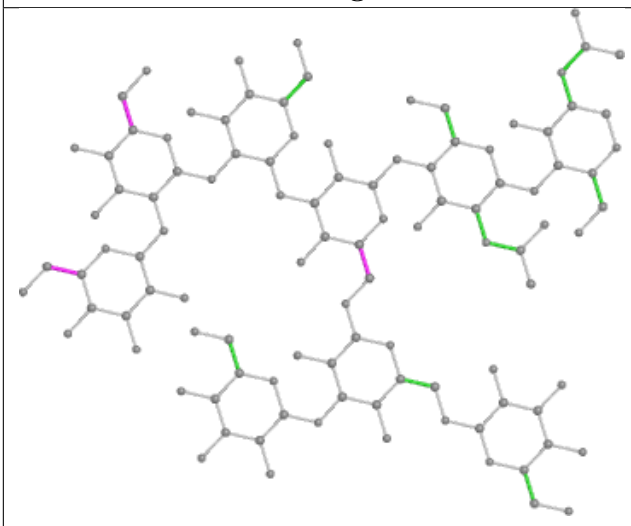
Oligosaccharide Chain I



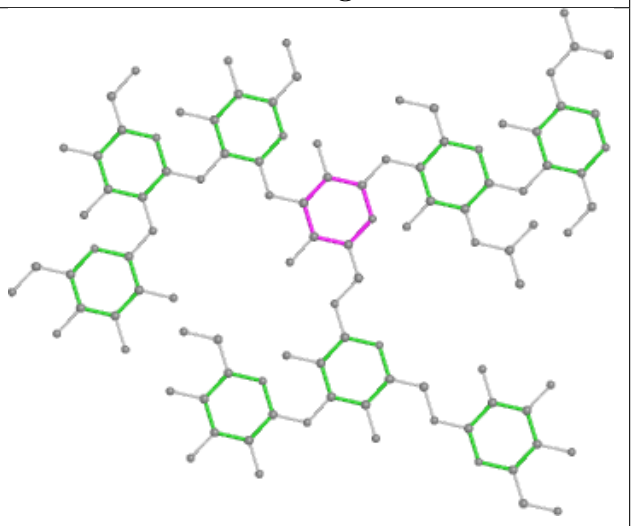
Bond lengths



Bond angles

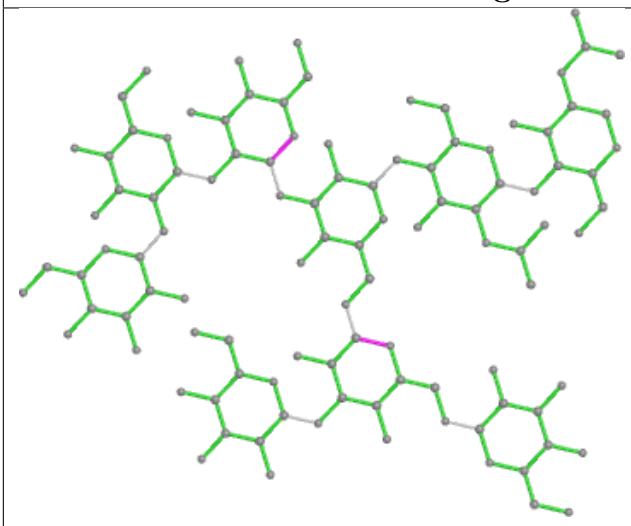


Torsions

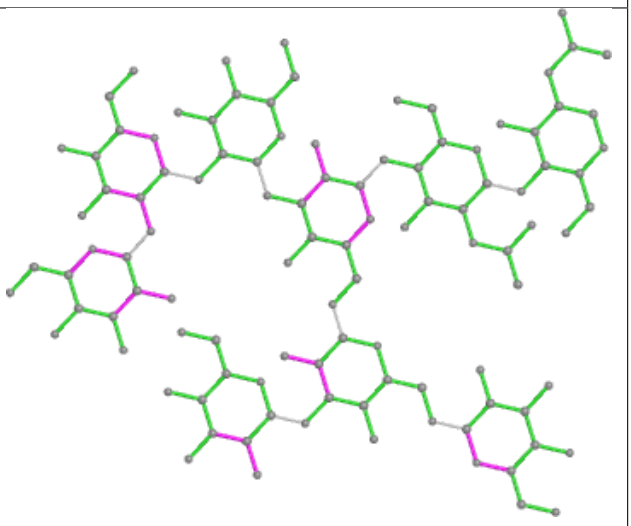


Rings

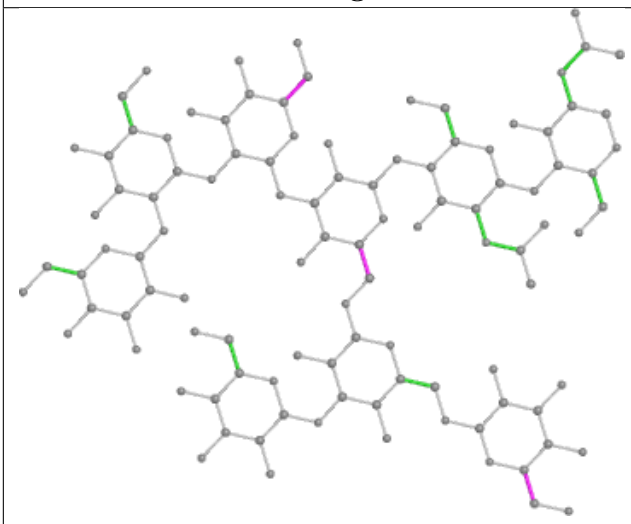
Oligosaccharide Chain N



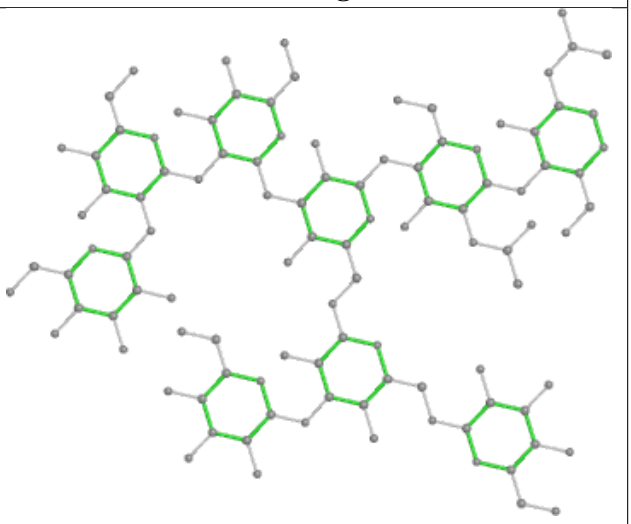
Bond lengths



Bond angles

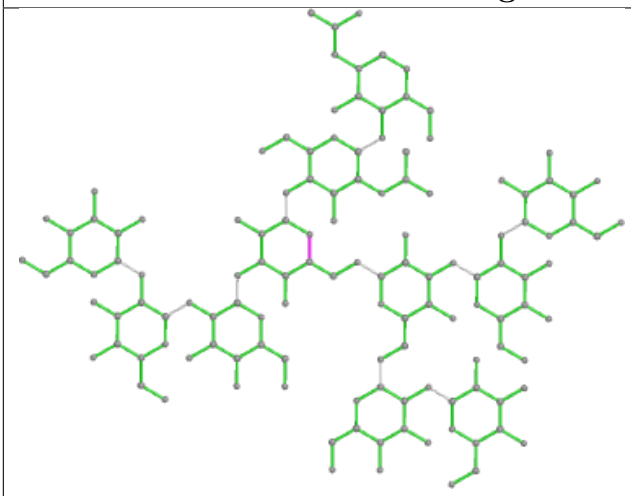


Torsions

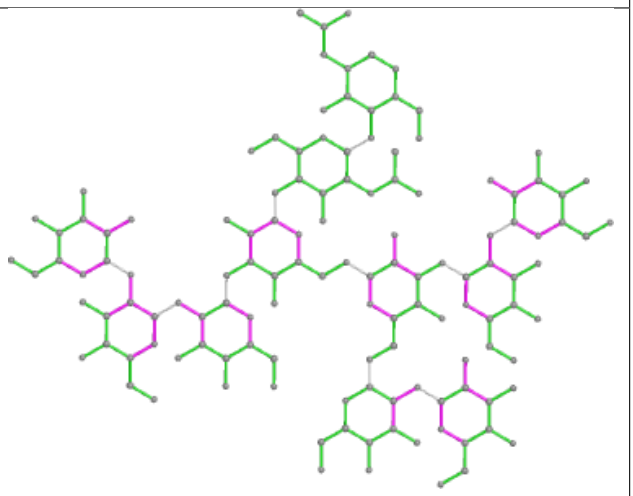


Rings

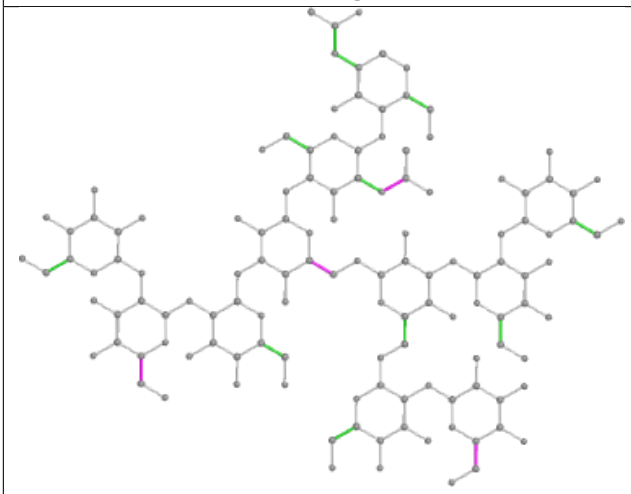
Oligosaccharide Chain J



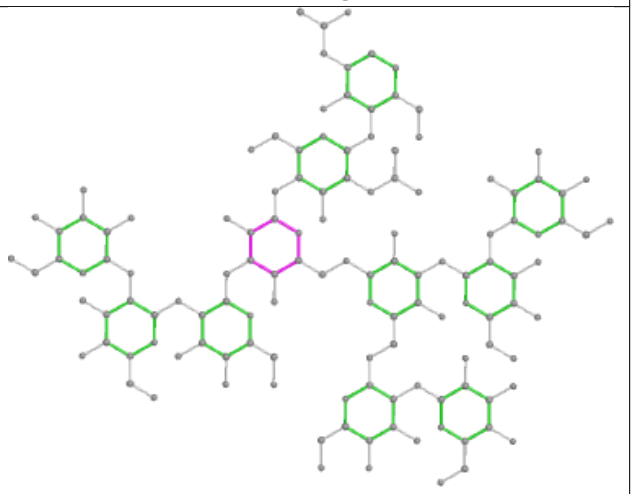
Bond lengths



Bond angles

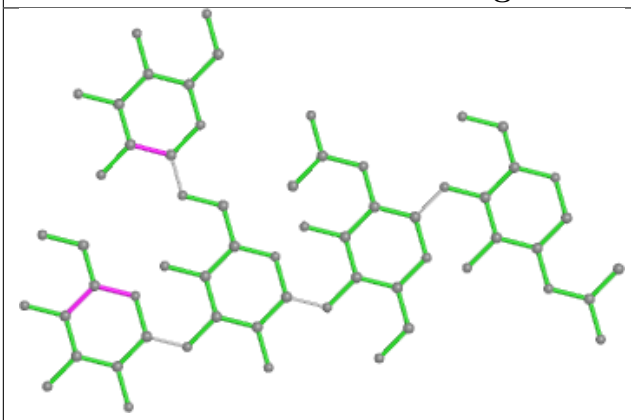


Torsions

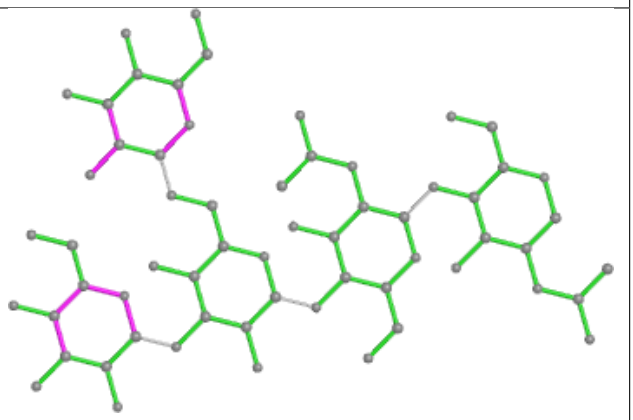


Rings

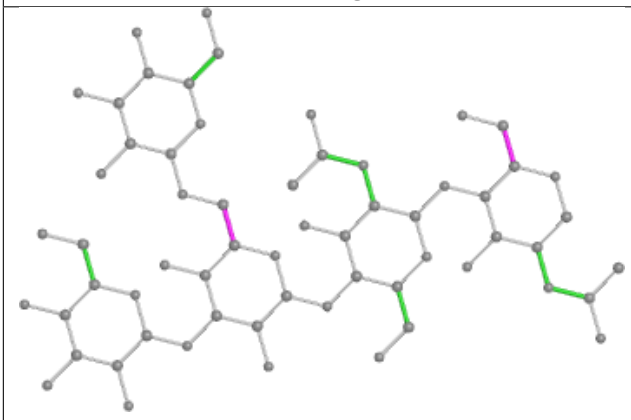
Oligosaccharide Chain K



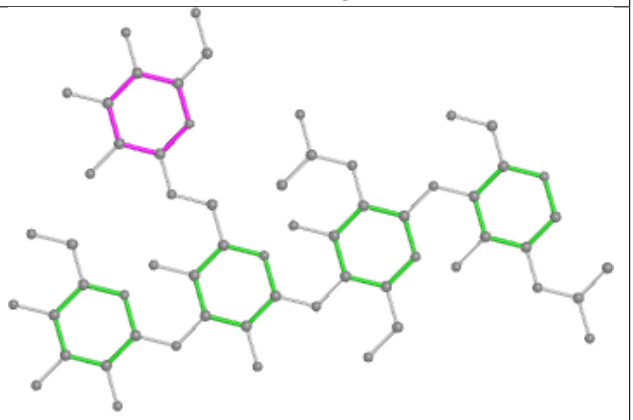
Bond lengths



Bond angles

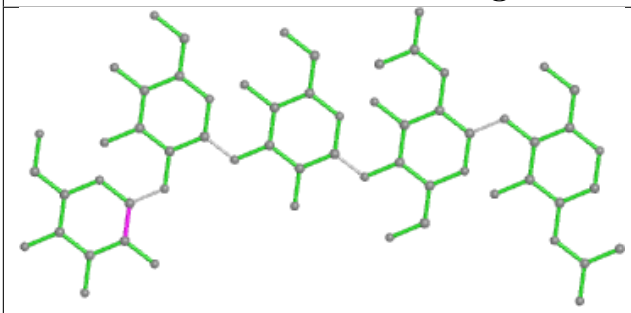


Torsions

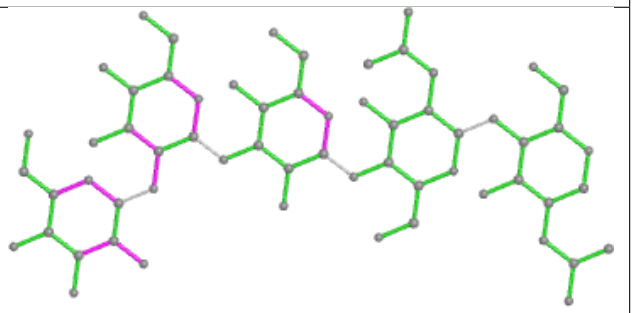


Rings

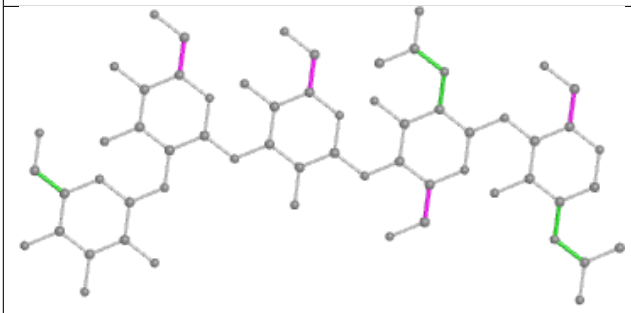
Oligosaccharide Chain M



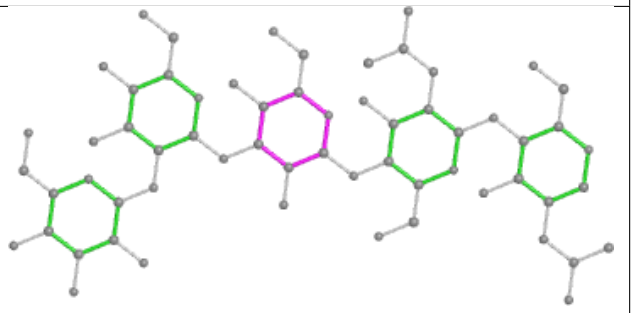
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	A	523	1	14,14,15	0.33	0	17,19,21	0.35	0
12	EDO	A	534	-	3,3,3	0.47	0	2,2,2	0.31	0
12	EDO	L	303	-	3,3,3	0.48	0	2,2,2	0.30	0
12	EDO	G	537	-	3,3,3	0.45	0	2,2,2	0.32	0
11	NAG	G	526	1	14,14,15	0.22	0	17,19,21	0.46	0
12	EDO	H	301	-	3,3,3	0.47	0	2,2,2	0.43	0
11	NAG	G	525	1	14,14,15	0.49	0	17,19,21	0.45	0
11	NAG	G	502	1	14,14,15	0.27	0	17,19,21	0.37	0
11	NAG	L	301	3	14,14,15	0.27	0	17,19,21	0.41	0
11	NAG	A	522	1	14,14,15	0.24	0	17,19,21	0.44	0
11	NAG	A	501	1	14,14,15	0.23	0	17,19,21	0.40	0
11	NAG	A	524	1	14,14,15	0.30	0	17,19,21	0.59	1 (5%)
11	NAG	C	301	3	14,14,15	0.21	0	17,19,21	0.41	0
12	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.28	0
11	NAG	A	521	1	14,14,15	0.16	0	17,19,21	0.39	0
12	EDO	L	302	-	3,3,3	0.49	0	2,2,2	0.28	0
11	NAG	G	527	1	14,14,15	0.37	0	17,19,21	0.36	0
11	NAG	A	512	1	14,14,15	0.20	0	17,19,21	0.54	0
11	NAG	G	501	1	14,14,15	0.18	0	17,19,21	0.33	0
13	ACT	B	303	-	3,3,3	0.77	0	3,3,3	1.33	0
11	NAG	G	514	1	14,14,15	0.42	0	17,19,21	0.65	1 (5%)
12	EDO	B	302	-	3,3,3	0.45	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	523	1	-	1/6/23/26	0/1/1/1
12	EDO	A	534	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EDO	L	303	-	-	0/1/1/1	-
12	EDO	G	537	-	-	0/1/1/1	-
11	NAG	G	526	1	-	2/6/23/26	0/1/1/1
12	EDO	H	301	-	-	1/1/1/1	-
11	NAG	G	525	1	-	2/6/23/26	0/1/1/1
11	NAG	G	502	1	-	2/6/23/26	0/1/1/1
11	NAG	L	301	3	-	0/6/23/26	0/1/1/1
11	NAG	A	522	1	-	0/6/23/26	0/1/1/1
11	NAG	A	501	1	-	2/6/23/26	0/1/1/1
11	NAG	A	524	1	-	2/6/23/26	0/1/1/1
11	NAG	C	301	3	-	0/6/23/26	0/1/1/1
12	EDO	B	301	-	-	0/1/1/1	-
11	NAG	A	521	1	-	0/6/23/26	0/1/1/1
12	EDO	L	302	-	-	0/1/1/1	-
11	NAG	G	527	1	-	2/6/23/26	0/1/1/1
11	NAG	A	512	1	-	3/6/23/26	0/1/1/1
11	NAG	G	501	1	-	2/6/23/26	0/1/1/1
11	NAG	G	514	1	-	1/6/23/26	0/1/1/1
12	EDO	B	302	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	514	NAG	C1-O5-C5	2.03	114.95	112.19
11	A	524	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	NAG	C4-C5-C6-O6
11	A	501	NAG	O5-C5-C6-O6
11	A	524	NAG	O5-C5-C6-O6
11	G	502	NAG	O5-C5-C6-O6
11	A	524	NAG	C4-C5-C6-O6
11	G	502	NAG	C4-C5-C6-O6
11	G	526	NAG	C4-C5-C6-O6
11	G	527	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	G	527	NAG	O5-C5-C6-O6
11	G	501	NAG	C4-C5-C6-O6
11	G	525	NAG	C1-C2-N2-C7
11	G	526	NAG	O5-C5-C6-O6
11	G	501	NAG	O5-C5-C6-O6
11	A	523	NAG	C4-C5-C6-O6
11	G	514	NAG	C3-C2-N2-C7
11	G	525	NAG	C3-C2-N2-C7
11	A	512	NAG	C4-C5-C6-O6
12	H	301	EDO	O1-C1-C2-O2
11	A	512	NAG	C3-C2-N2-C7
11	A	512	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	523	NAG	1	0
12	G	537	EDO	2	0
11	A	501	NAG	2	0
12	B	301	EDO	1	0
11	G	527	NAG	1	0
12	B	302	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	337/344 (97%)	1.47	90 (26%) 0 0	66, 116, 187, 209	0
1	G	333/344 (96%)	0.57	33 (9%) 7 8	48, 93, 136, 171	0
2	B	225/229 (98%)	0.43	20 (8%) 9 10	48, 79, 148, 183	0
2	H	221/229 (96%)	0.45	19 (8%) 10 11	30, 63, 136, 171	0
3	C	219/219 (100%)	0.39	11 (5%) 28 31	37, 67, 140, 198	0
3	L	218/219 (99%)	0.41	17 (7%) 13 14	34, 63, 144, 181	0
All	All	1553/1584 (98%)	0.68	190 (12%) 4 4	30, 87, 158, 209	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	10.1
1	A	44	VAL	9.8
1	A	198	GLY	9.2
1	A	491	ILE	9.0
1	A	225	ILE	8.3
1	A	244	SER	8.1
1	A	223	TYR	7.5
1	A	89	VAL	7.4
1	A	45	TRP	7.3
2	B	138	LEU	7.2
2	H	189	LEU	7.2
1	A	217	TYR	6.6
1	A	91	GLU	6.3
1	A	90	THR	5.9
3	C	214	CYS	5.8
1	A	52	LEU	5.7
1	A	245	VAL	5.6
1	A	461	ASN	5.5
1	A	224	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	HIS	5.2
1	A	60	ALA	5.2
3	C	150	VAL	5.0
3	C	209	PHE	4.9
2	B	125	ALA	4.7
2	B	189	LEU	4.7
1	A	239	CYS	4.6
3	L	213	GLU	4.5
2	H	195	ILE	4.3
1	A	247	CYS	4.3
2	H	159	LEU	4.3
1	A	220	PRO	4.2
3	C	192	TYR	4.2
1	A	357	LYS	4.2
1	G	87	VAL	4.2
1	A	324	GLY	4.1
1	A	87	VAL	4.1
1	G	353	PHE	4.1
2	H	191	THR	4.1
3	L	191	VAL	4.0
1	A	221	ALA	4.0
1	A	254	VAL	4.0
1	A	488	VAL	3.9
1	A	492	GLU	3.9
1	A	462	ASN	3.9
1	A	246	GLN	3.9
1	A	80	ASN	3.9
1	A	489	VAL	3.9
3	L	209	PHE	3.8
1	A	93	PHE	3.8
2	B	130	SER	3.7
1	A	53	PHE	3.6
1	A	75	VAL	3.6
1	G	367	GLY	3.6
3	L	125	LEU	3.6
3	L	150	VAL	3.6
1	A	459	GLY	3.6
2	B	193	THR	3.6
2	B	211	VAL	3.5
1	A	81	PRO	3.5
2	H	154	TRP	3.5
1	A	352	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	156	SER	3.5
1	A	55	ALA	3.4
3	C	187	GLU	3.4
1	A	79	PRO	3.4
1	A	78	ASP	3.4
2	H	128	SER	3.4
2	H	124	LEU	3.4
2	H	211	VAL	3.3
2	B	131	THR	3.3
2	B	214	LYS	3.3
1	A	51	THR	3.3
1	A	218	CYS	3.3
1	A	83	GLU	3.3
1	A	59	LYS	3.3
1	A	227	LYS	3.3
1	A	48	ALA	3.2
1	A	219	THR	3.2
3	L	192	TYR	3.2
1	G	277	LEU	3.2
2	H	190	GLY	3.2
1	A	255	VAL	3.1
1	A	77	THR	3.1
1	G	44	VAL	3.1
1	G	124	GLY	3.1
1	A	350	LYS	3.1
1	G	430	VAL	3.0
2	B	194	TYR	3.0
3	L	122	ASP	3.0
3	C	152	ASN	3.0
2	B	158	ALA	3.0
1	A	46	ARG	3.0
2	H	138	LEU	2.9
2	H	194	TYR	2.9
1	A	238	PRO	2.9
1	A	50	THR	2.9
1	A	349	LEU	2.8
1	A	354	ASN	2.8
1	A	277	LEU	2.8
2	B	123	PRO	2.8
1	G	255	VAL	2.8
1	A	398	SER	2.7
2	H	186	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	118	PHE	2.7
1	A	201	ILE	2.7
1	G	458	GLY	2.7
1	A	226	LEU	2.7
3	C	183	LYS	2.7
3	L	190	LYS	2.7
1	G	324	GLY	2.7
1	G	122	LEU	2.7
1	A	351	GLU	2.6
1	G	242	VAL	2.6
1	G	221	ALA	2.6
3	C	184	ALA	2.6
1	A	269	GLU	2.6
1	A	353	PHE	2.5
2	H	193	THR	2.5
1	G	376	PHE	2.5
1	A	85	HIS	2.5
1	A	199	SER	2.5
3	L	88	CYS	2.5
1	A	490	GLU	2.5
1	A	233	PHE	2.5
1	A	72	HIS	2.5
1	G	352	HIS	2.5
1	A	202	LYS	2.4
3	L	210	ASN	2.4
1	A	452	ILE	2.4
1	A	243	SER	2.4
3	L	179	LEU	2.4
2	H	185	PRO	2.4
1	G	46	ARG	2.4
1	A	229	ASN	2.4
1	A	47	ASP	2.4
1	G	257	THR	2.4
1	G	349	LEU	2.4
1	A	54	CYS	2.4
3	C	126	LYS	2.3
1	G	85	HIS	2.3
1	A	358	THR	2.3
2	B	124	LEU	2.3
3	L	132	VAL	2.3
3	L	180	THR	2.3
1	G	350	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	118	PHE	2.3
1	A	92	ASN	2.3
2	H	158	ALA	2.3
1	G	89	VAL	2.3
2	B	127	SER	2.3
2	B	190	GLY	2.2
3	L	186	TYR	2.2
1	A	76	PRO	2.2
1	G	464	SER	2.2
2	B	208	ASP	2.2
3	L	151	ASP	2.2
2	H	212	GLU	2.2
1	A	487	LYS	2.2
1	G	240	LYS	2.2
1	A	260	LEU	2.2
1	A	99	LYS	2.2
2	B	207	VAL	2.2
1	A	49	ASP	2.2
1	A	71	THR	2.2
1	A	62	GLU	2.2
1	A	228	CYS	2.2
1	A	326	ILE	2.2
1	G	449	ILE	2.2
1	G	45	TRP	2.2
1	G	224	VAL	2.1
1	A	365	SER	2.1
1	G	487	LYS	2.1
2	B	154	TRP	2.1
2	H	127	SER	2.1
1	G	374	HIS	2.1
2	H	160	THR	2.1
3	C	122	ASP	2.1
1	G	82	GLN	2.1
1	A	256	SER	2.1
1	G	260	LEU	2.1
3	L	184	ALA	2.1
1	A	124	GLY	2.1
1	G	301	ASN	2.1
2	B	187	SER	2.1
1	G	93	PHE	2.1
2	B	152	VAL	2.0
1	A	116	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	478	ASN	2.0
2	B	213	PRO	2.0
1	G	281	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MAN	K	4	11/12	0.58	0.39	136,142,145,149	0
9	MAN	K	3	11/12	0.71	0.37	128,134,140,145	0
5	NAG	E	2	14/15	0.74	0.40	142,146,149,151	0
10	MAN	M	5	11/12	0.75	0.40	88,101,109,112	0
6	MAN	F	6	11/12	0.78	0.30	111,120,129,134	0
9	MAN	K	5	11/12	0.82	0.38	132,136,138,139	0
6	MAN	F	5	11/12	0.82	0.55	109,119,128,131	0
5	NAG	E	1	14/15	0.83	0.28	99,120,127,135	0
8	MAN	J	5	11/12	0.83	0.13	82,89,105,119	0
7	MAN	N	5	11/12	0.84	0.12	59,72,78,81	0
9	NAG	K	1	14/15	0.84	0.20	67,83,100,100	0
6	NAG	F	2	14/15	0.85	0.21	92,97,102,104	0
9	NAG	K	2	14/15	0.85	0.20	65,98,109,118	0
10	NAG	M	2	14/15	0.85	0.18	76,89,97,98	0
8	MAN	J	6	11/12	0.85	0.19	108,125,126,127	0
4	MAN	D	10	11/12	0.86	0.19	119,124,129,130	0
10	NAG	M	1	14/15	0.87	0.13	70,83,92,93	0
7	MAN	N	9	11/12	0.87	0.13	72,79,84,86	0
7	MAN	I	7	11/12	0.87	0.12	66,86,93,101	0
7	MAN	N	6	11/12	0.88	0.27	54,87,91,95	0
10	MAN	M	3	11/12	0.88	0.20	77,83,86,87	0
4	MAN	D	9	11/12	0.88	0.13	76,83,91,105	0
7	MAN	I	4	11/12	0.89	0.14	97,107,112,113	0
4	MAN	D	7	11/12	0.90	0.13	65,69,75,78	0
4	MAN	D	6	11/12	0.90	0.17	86,91,96,99	0

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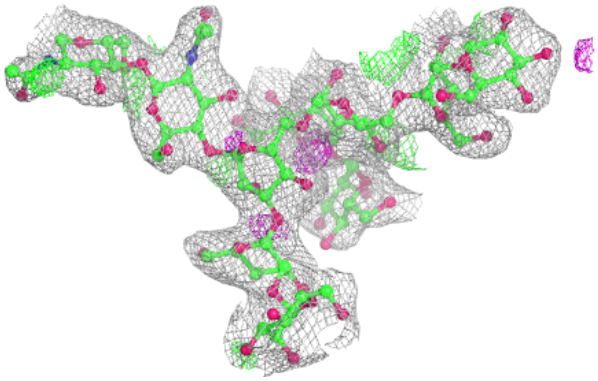
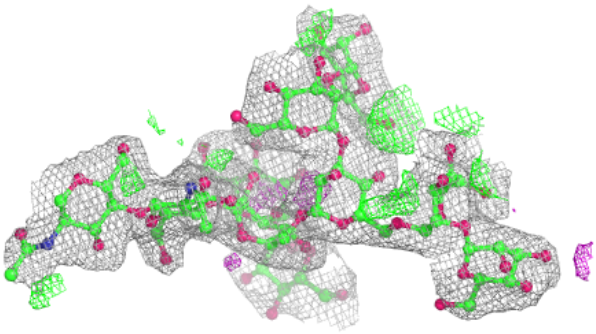
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MAN	M	4	11/12	0.90	0.14	50,71,78,91	0
6	MAN	F	3	11/12	0.90	0.15	81,96,106,116	0
7	MAN	I	8	11/12	0.91	0.12	100,111,116,119	0
7	MAN	I	3	11/12	0.91	0.12	66,78,85,87	0
4	MAN	D	3	11/12	0.91	0.16	56,65,75,81	0
6	MAN	F	4	11/12	0.91	0.14	66,74,86,97	0
7	MAN	I	5	11/12	0.92	0.19	77,92,101,102	0
6	NAG	F	1	14/15	0.92	0.13	61,75,94,95	0
7	NAG	N	1	14/15	0.93	0.16	41,50,56,57	0
7	MAN	I	9	11/12	0.93	0.13	82,91,95,96	0
8	MAN	J	3	11/12	0.93	0.13	35,42,56,59	0
7	MAN	I	6	11/12	0.94	0.21	74,83,91,94	0
7	NAG	I	2	14/15	0.94	0.13	57,72,83,89	0
7	MAN	N	7	11/12	0.94	0.10	54,57,72,75	0
7	MAN	N	8	11/12	0.94	0.11	84,88,96,98	0
4	NAG	D	2	14/15	0.94	0.12	64,68,76,82	0
4	MAN	D	5	11/12	0.94	0.13	61,64,84,85	0
8	MAN	J	4	11/12	0.94	0.12	68,75,86,93	0
7	NAG	I	1	14/15	0.94	0.15	42,64,73,78	0
7	MAN	N	4	11/12	0.94	0.12	71,73,85,89	0
8	MAN	J	9	11/12	0.94	0.11	47,52,64,64	0
8	MAN	J	7	11/12	0.95	0.16	36,38,43,46	0
4	MAN	D	4	11/12	0.95	0.13	56,59,66,68	0
8	NAG	J	2	14/15	0.96	0.14	29,51,58,64	0
4	NAG	D	1	14/15	0.96	0.17	44,59,83,89	0
8	MAN	J	10	11/12	0.96	0.13	33,40,45,47	0
8	MAN	J	11	11/12	0.96	0.13	48,51,63,71	0
4	MAN	D	8	11/12	0.96	0.14	66,71,85,92	0
7	NAG	N	2	14/15	0.96	0.13	44,49,53,59	0
8	NAG	J	1	14/15	0.96	0.19	37,45,50,51	0
8	MAN	J	8	11/12	0.97	0.16	44,48,53,54	0
7	MAN	N	3	11/12	0.98	0.11	50,59,64,66	0

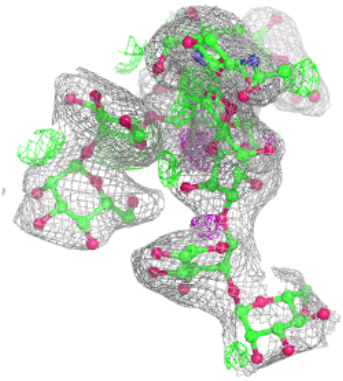
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

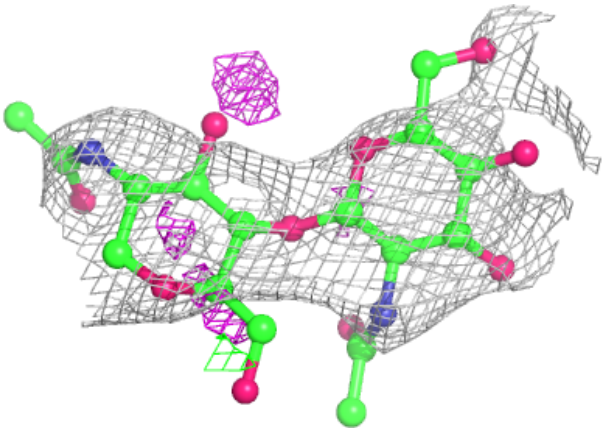


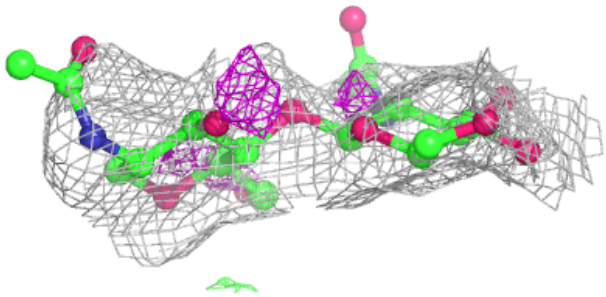


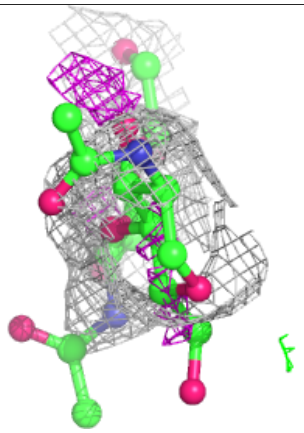


Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

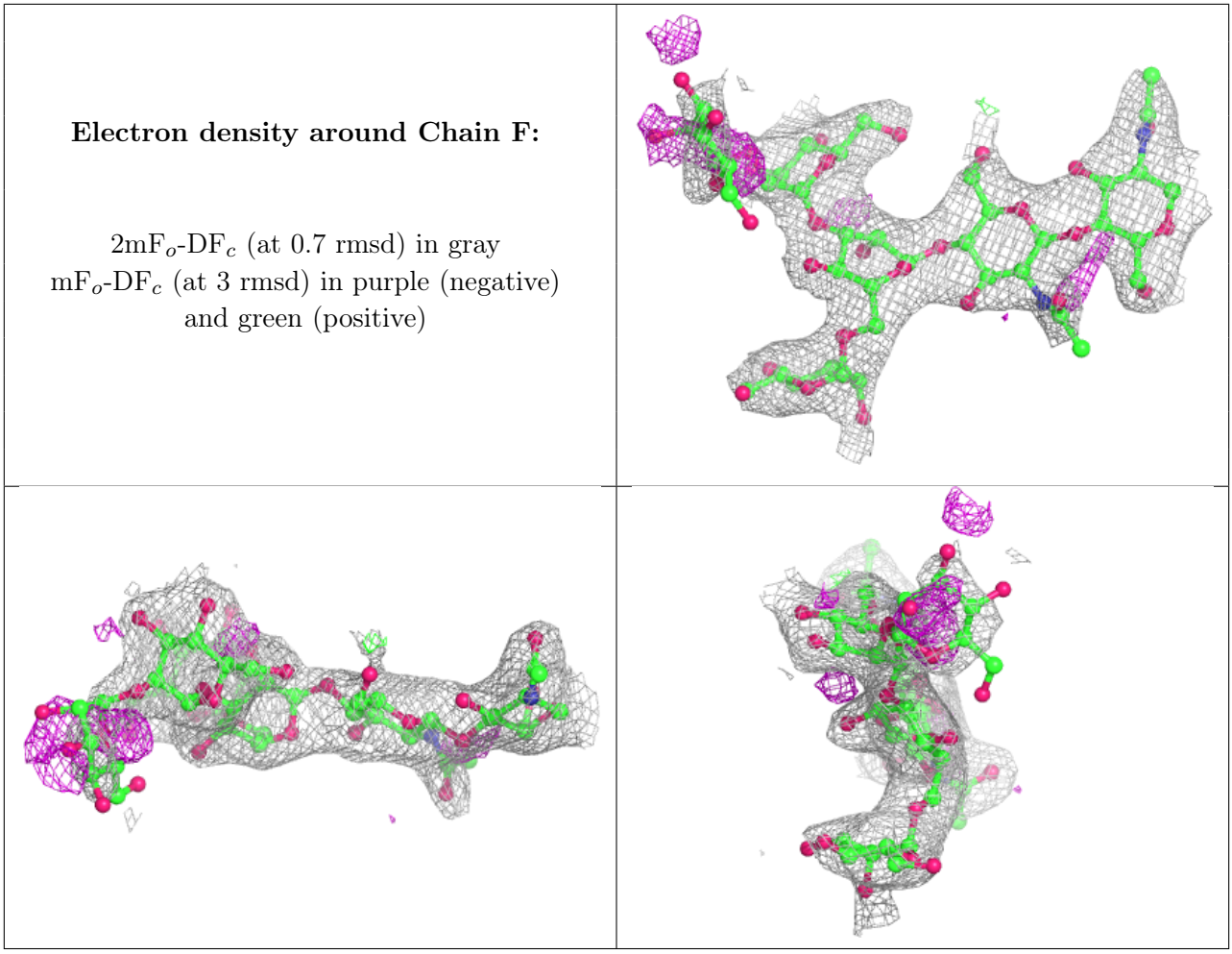






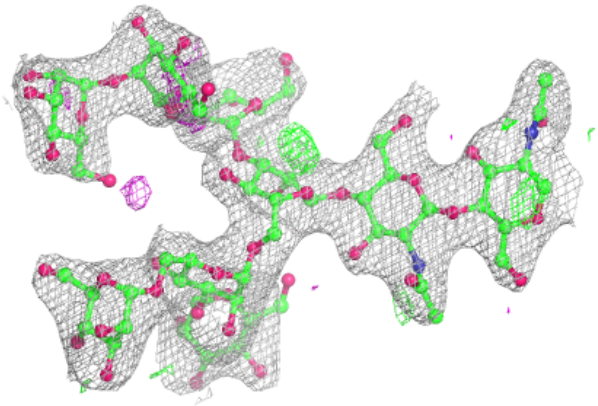
Electron density around Chain F:

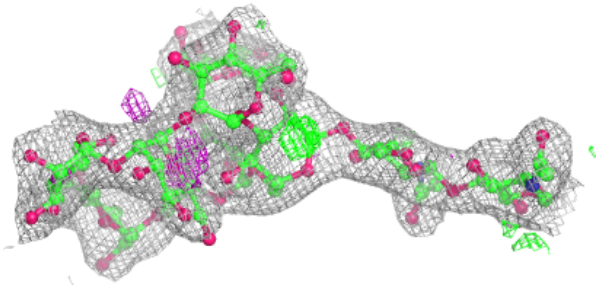
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

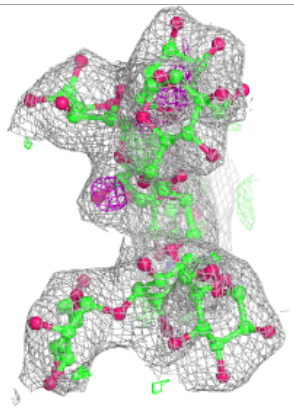


Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

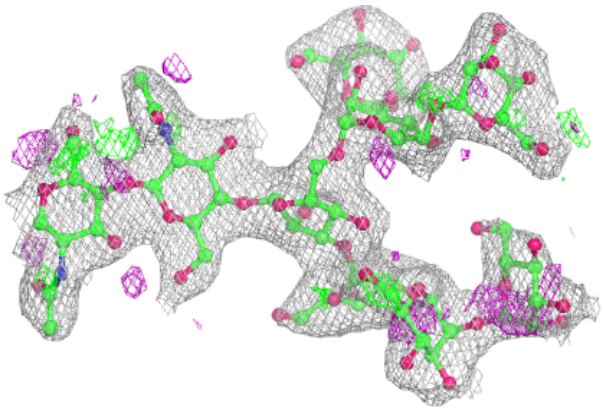


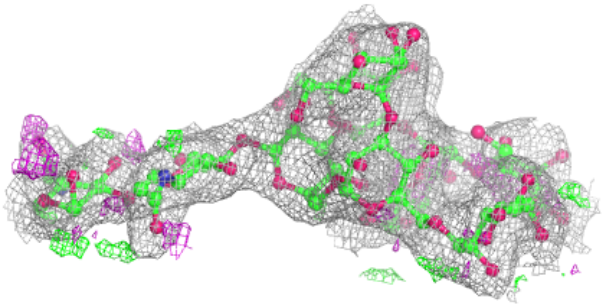


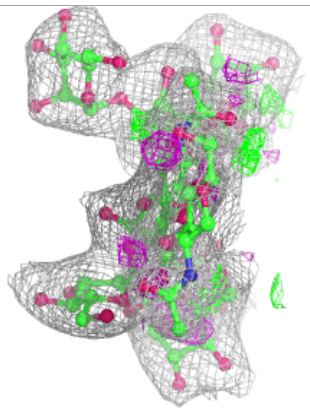


Electron density around Chain N:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

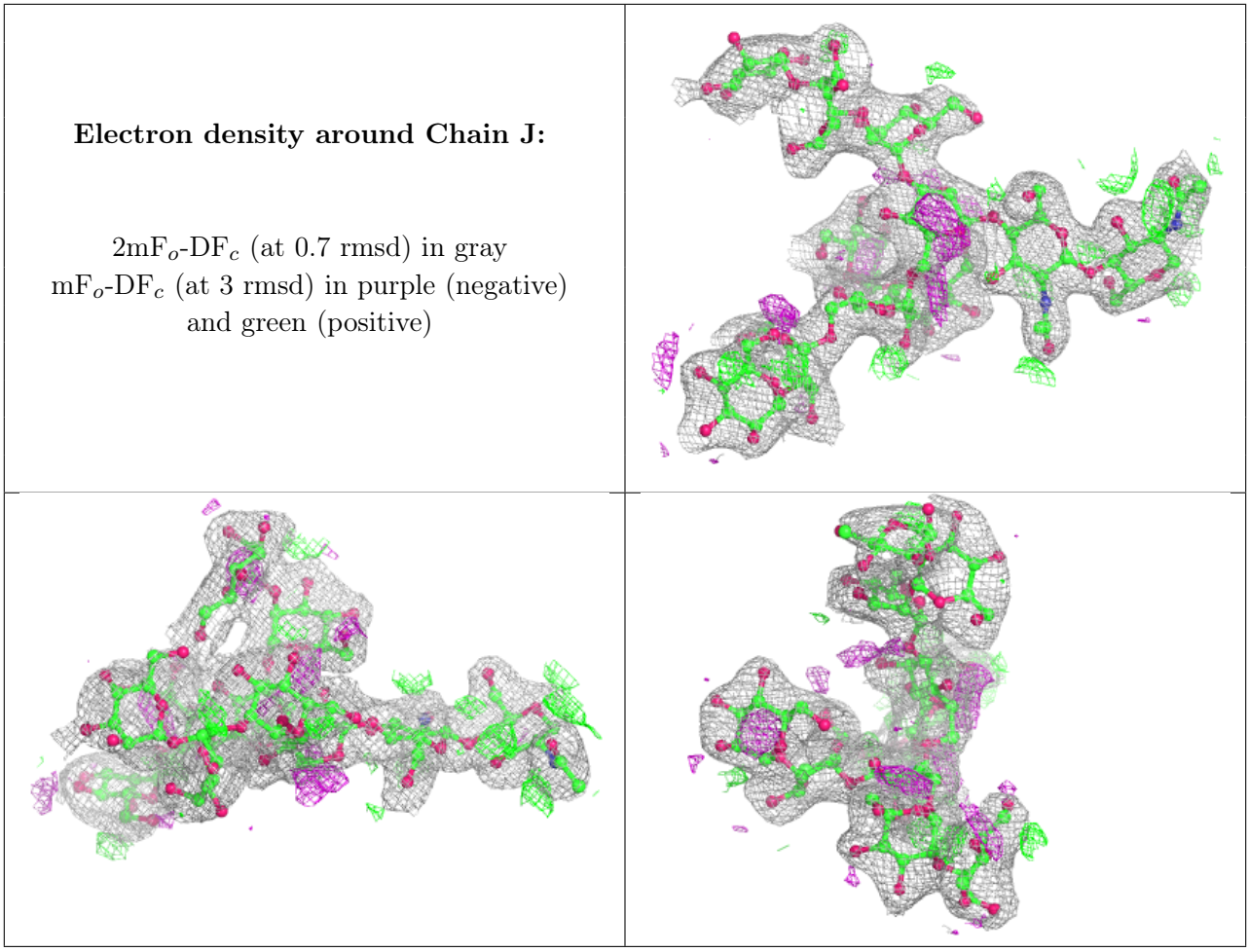






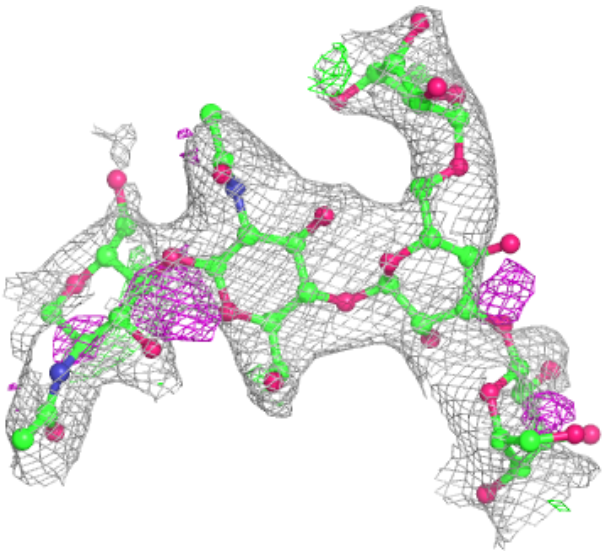
Electron density around Chain J:

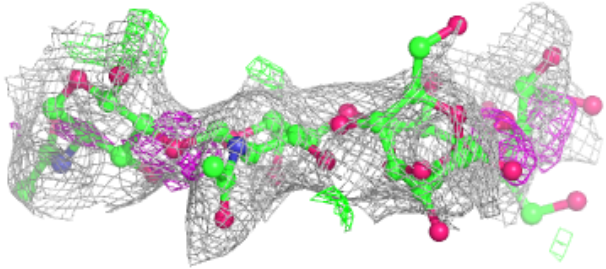
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

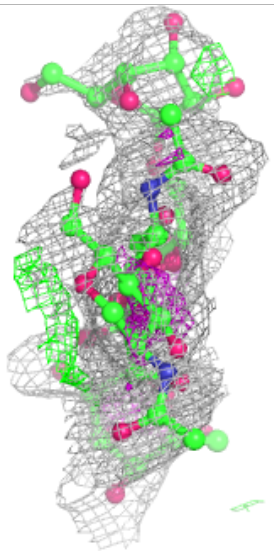


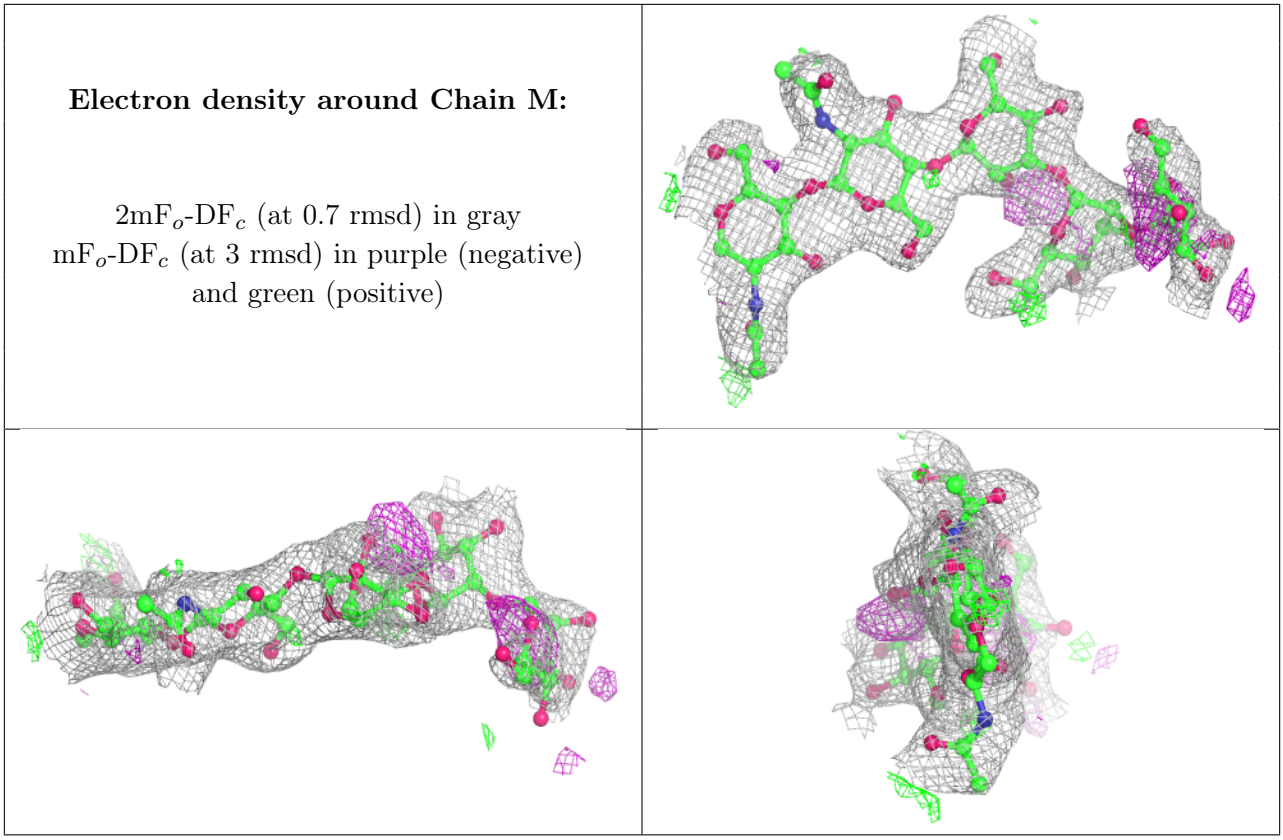
Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)









6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	G	502	14/15	0.50	0.46	101,124,133,135	0
12	EDO	L	303	4/4	0.60	0.33	76,89,97,97	0
11	NAG	A	524	14/15	0.65	0.55	118,135,139,142	0
12	EDO	G	537	4/4	0.71	0.34	64,66,68,73	0
11	NAG	G	525	14/15	0.76	0.29	94,108,114,117	0
11	NAG	G	514	14/15	0.79	0.20	87,100,115,123	0
11	NAG	A	521	14/15	0.79	0.31	99,114,127,131	0
11	NAG	A	512	14/15	0.81	0.36	103,120,126,128	0
11	NAG	A	501	14/15	0.85	0.52	109,134,144,150	0
12	EDO	H	301	4/4	0.85	0.24	57,62,64,70	0
12	EDO	L	302	4/4	0.85	0.32	73,74,75,76	0
12	EDO	B	302	4/4	0.85	0.17	94,94,95,96	0
11	NAG	G	527	14/15	0.88	0.16	67,88,105,107	0
11	NAG	G	526	14/15	0.88	0.21	54,86,110,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	EDO	B	301	4/4	0.89	0.22	78,84,87,88	0
11	NAG	A	523	14/15	0.89	0.24	88,101,104,107	0
13	ACT	B	303	4/4	0.89	0.18	82,88,90,90	0
12	EDO	A	534	4/4	0.90	0.13	99,99,101,103	0
11	NAG	A	522	14/15	0.90	0.10	67,76,82,89	0
11	NAG	G	501	14/15	0.91	0.18	81,98,119,122	0
11	NAG	C	301	14/15	0.97	0.10	57,62,72,76	0
11	NAG	L	301	14/15	0.97	0.10	34,57,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.